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New Prebiotic Molecules in the Interstellar Medium from the Reaction Between Vinyl Alcohol and CN Radical†: Unsupervised Reaction Mechanism Discovery, Accurate Electronic Structure Calculations and Kinetic Simulations

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Contents

1 Supporting Information

Here are reported the cartesian coordinates of each optimized structures involved in the two reactions: *syn*-VyA + CN and *anti*-VyA + CN.

2 Cartesian coordinates

2.1 Addition reactions

2.1.1 *syn*-VyA + CN

CN (Cyanide radical)

Table 1 Cartesian coordinates in Å of the cyanide radical structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−1.875383	0.453789	0.017829
N	−0.716421	0.453789	0.017829

C_2H_4O (*syn*-VyA)

Table 2 Cartesian coordinates in Å of the *syn*-VyA structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.036309	0.442827	0.000002
O	1.206308	−0.115176	−0.000002
H	0.027835	1.523455	−0.000001
C	−1.199885	−0.207586	0.000001
H	−1.253910	−1.290335	−0.000002
H	−2.123655	0.351690	−0.000006
H	1.116437	−1.074853	0.000005

s-Int1

Table 3 Cartesian coordinates in Å of the **s-Int1** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−1.223970	0.346877	0.284567
O	−1.480884	−0.913455	−0.162057
H	−2.121561	0.940412	0.387136
C	0.040897	1.030829	−0.153977
H	0.211418	1.921086	0.454209
H	−0.010268	1.353709	−1.203771
H	−0.655988	−1.414046	−0.216449
C	1.190800	0.128598	−0.026067
N	2.045701	−0.651991	0.057004

s-Int1b

Table 4 Cartesian coordinates in Å of the **s-Int1b** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.608031	0.077743	0.482179
O	1.603376	−0.532773	−0.264103
H	0.753870	0.115309	1.558569
C	−0.101622	1.228876	−0.170371
H	0.174886	1.443105	−1.195982
H	−0.398541	2.070548	0.443327
H	1.599009	−1.476259	−0.070555
C	−0.848535	−0.058934	0.027189
N	−1.819387	−0.773261	−0.085589

s-Int2

Table 5 Cartesian coordinates in Å of the **s-Int2** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.424723	−0.018446	0.383703
O	1.006460	−1.208950	−0.140369
H	0.560788	−0.108137	1.466272
C	1.086852	1.217589	−0.126004
H	2.154941	1.311218	0.005584
H	0.522218	2.012839	−0.587756
H	0.992787	−1.145271	−1.102593
C	−1.033056	0.018850	0.124049
N	−2.170629	0.053585	−0.102315

s-Int3

Table 6 Cartesian coordinates in Å of the **s-Int3** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.988855	−0.451602	0.291772
O	2.181772	0.091644	−0.250676
H	0.700065	−1.384477	−0.203082
C	−0.141240	0.528383	0.246121
H	0.057252	1.572710	0.446049
H	2.046477	0.238001	−1.192277
C	−1.461617	0.120365	0.020576
N	−2.547823	−0.241163	−0.175942
H	1.225660	−0.692625	1.332968

s-Int4

Table 7 Cartesian coordinates in Å of the **s-Int4** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.338179	0.053219	0.000062
O	0.862528	1.306811	0.000292
C	1.325205	−1.052983	0.000045
H	1.968304	−0.991214	0.883150
H	0.816834	−2.015413	−0.000143
H	0.152117	1.959414	0.000287
C	−1.050149	−0.116959	−0.000144
N	−2.208459	−0.235861	−0.000314
H	1.968528	−0.990987	−0.882881

s-Int5

Table 8 Cartesian coordinates in Å of the **s-Int5** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.409848	−0.041316	0.380390
O	1.041703	−1.144416	−0.140658
C	1.125194	1.214977	−0.154543
H	1.065265	1.238867	−1.241852
H	0.635570	2.101157	0.248889
C	−1.038927	0.003264	0.057753
N	−2.171740	0.059832	−0.186926
H	2.168228	1.191981	0.156014
H	0.521602	−0.063452	1.472807

s-TS1

Table 9 Cartesian coordinates in Å of the **s-TS1** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.667077	0.096591	0.485498
O	1.634643	−0.636635	−0.148131
H	0.807100	0.126835	1.556499
C	−0.094898	1.197815	−0.185872
H	0.167373	1.426518	−1.215603
H	−0.355272	2.063858	0.415481
H	1.427359	−0.716241	−1.085950
C	−0.934516	−0.001828	−0.000229
N	−1.827872	−0.791445	−0.050937

s-TS1b

Table 10 Cartesian coordinates in Å of the **s-TS1b** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.579745	0.065395	0.458799
O	1.577886	−0.582191	−0.265314
H	0.740393	0.115893	1.535460
C	0.020950	1.289451	−0.169491
H	0.192060	1.436633	−1.225814
H	−0.304558	2.112406	0.449097
H	1.542735	−1.523286	−0.062155
C	−0.829581	−0.182495	0.091930
N	−1.904478	−0.640018	−0.123799

s-TS3

Table 11 Cartesian coordinates in Å of the **s-TS3** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	1.250669	0.421444	−0.080454
O	1.448643	−0.922534	−0.134443
H	2.114504	1.008116	0.195654
C	−0.102803	0.996542	0.152658
H	0.500170	1.057870	−0.988633
H	−0.181906	1.956790	0.641123
H	0.610965	−1.384199	0.013819
C	−1.210093	0.115617	0.129903
N	−2.059686	−0.679345	0.077561

s-TS3b

Table 12 Cartesian coordinates in Å of the **s-TS3b** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.255727	0.377936	0.511840
O	1.217745	−1.312316	−0.036073
H	0.515450	0.158045	1.537357
C	1.023432	1.184436	−0.249777
H	0.702847	1.496782	−1.234800
H	1.999153	1.490612	0.098749
H	1.018149	−1.323017	−0.985933
C	−1.099169	0.063911	0.121422
N	−2.190669	−0.166943	−0.188721

s-TS4

Table 13 Cartesian coordinates in Å of the **s-TS4** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	1.218794	0.359823	0.129795
O	1.447658	−0.937661	−0.082283
H	2.129943	0.922701	0.278346
C	0.007550	0.967935	0.082590
H	−0.255485	1.534396	−1.637180
H	−0.090116	1.995308	0.398433
H	0.608169	−1.408334	−0.201017
C	−1.162855	0.135973	0.051064
N	−2.045135	−0.617700	0.023905

s-TS5

Table 14 Cartesian coordinates in Å of the **s-TS5** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.911418	−0.314912	−0.087016
O	−2.187371	0.126116	−0.081448
H	−0.811696	−1.154395	1.549218
C	0.104414	0.552000	0.111747
H	−0.085893	1.574247	0.408131
H	−2.789749	−0.616243	−0.187521
C	1.452092	0.102200	0.004034
N	2.550544	−0.258025	−0.080419
H	−0.725060	−1.309320	−0.478730

s-TS8

Table 15 Cartesian coordinates in Å of the **s-TS8** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	1.267046	0.339467	0.113826
O	1.434166	−0.873503	0.112479
H	2.120280	1.027310	0.197248
C	−0.071833	1.002080	−0.112612
H	−0.063410	1.449299	−1.115315
H	−0.193053	1.828586	0.593385
H	1.477279	−1.623256	−1.150525
C	−1.204727	0.085736	−0.004447
N	−2.115708	−0.626082	0.082118

s-TS10

Table 16 Cartesian coordinates in Å of the **s-TS10** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.302171	−0.068947	0.490469
O	0.997951	−1.130198	−0.185764
H	0.385532	−0.151275	1.574392
C	1.221740	0.927431	−0.157514
H	0.828727	1.513614	−0.979728
H	1.998643	1.360990	0.460350
H	1.704876	−0.199318	−0.678716
C	−1.111398	0.022089	0.103609
N	−2.229604	0.112745	−0.193324

s-TS12

Table 17 Cartesian coordinates in Å of the **s-TS12** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.334038	−0.054029	0.133156
O	0.929903	−1.280255	−0.049322
H	0.732929	0.651726	1.118530
C	1.132907	1.179164	−0.041148
H	0.638686	2.112256	−0.261441
H	2.206066	1.076333	−0.087525
H	1.472745	−1.238061	−0.848368
C	−1.091167	0.006170	0.023773
N	−2.249515	0.075763	−0.029666

s-TS13

Table 18 Cartesian coordinates in Å of the **s-TS13** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.404534	0.110560	0.080546
O	0.933802	1.210862	0.154848
C	1.145341	−1.181204	−0.032381
H	2.198169	−1.021530	0.189752
H	0.716415	−1.928851	0.637712
H	1.425798	1.899735	−1.094031
C	−1.063633	0.018064	0.003480
N	−2.214645	−0.085852	−0.057717
H	1.036995	−1.560560	−1.054883

s-TS14

Table 19 Cartesian coordinates in Å of the **s-TS14** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.427525	0.205295	0.055679
O	−0.882098	1.320709	−0.116335
C	−1.236125	−1.069884	−0.062106
H	−1.198752	−1.372550	−1.112793
H	−0.815043	−1.873649	0.540853
C	1.052554	−0.007870	0.004781
N	2.195794	−0.202452	−0.061282
H	−2.268772	−0.870287	0.216498
H	−0.364628	0.202725	1.724963

s-TS15

Table 20 Cartesian coordinates in Å of the **s-TS15** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.310687	0.527182	0.408540
O	−0.868530	1.354743	−0.294369
C	−1.281700	−1.294700	−0.095820
H	−1.035936	−1.322914	−1.148311
H	−0.764334	−1.986617	0.557108
C	1.047279	0.024054	0.078946
N	2.112807	−0.374459	−0.155865
H	−2.289028	−1.004616	0.168934
H	−0.591439	0.351855	1.457777

s-TS16

Table 21 Cartesian coordinates in Å of the **s-TS16** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.436290	0.033779	0.059402
O	0.996474	−1.197203	−0.142723
H	0.329343	−0.013623	1.856427
C	1.172628	1.151842	−0.077762
H	0.693242	2.117949	−0.053825
H	2.248480	1.081821	−0.148338
H	0.412434	−1.880038	0.205614
C	−1.015941	0.089477	−0.006934
N	−2.172698	0.084454	−0.074650

s-P1 (cyanovinylalcohol isomer + H)

Table 22 Cartesian coordinates in Å of the cyanovinylalcohol isomer structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.928205	−0.382036	0.000000
H	−0.737944	−1.447545	0.000000
C	0.066381	0.520301	0.000000
H	−0.130291	1.586302	0.000000
O	−2.245078	−0.107506	0.000000
H	−2.383240	0.847574	−0.000000
C	1.427541	0.100522	0.000000
N	2.545400	−0.222715	−0.000000

s-P2 (cyanovinylalcohol isomer + H)

Table 23 Cartesian coordinates in Å of the cyanovinylalcohol isomer structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.443981	0.039262	−0.000001
C	1.198529	1.140439	0.000000
H	2.276862	1.062360	0.000002
O	0.990152	−1.212171	−0.000000
H	0.291376	−1.874294	0.000005
C	−0.994930	0.104485	−0.000001
N	−2.157744	0.098859	0.000001
H	0.729281	2.112173	0.000000

s-P3 (cyanoacetaldehyde + H)

Table 24 Cartesian coordinates in Å of the cyanoacetaldehyde structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−1.345923	0.104809	−0.027948
N	−2.377393	−0.417343	−0.125136
C	−0.023598	0.714489	0.099916
H	0.191721	1.363573	−0.749015
H	−0.003508	1.324207	1.009576
C	1.076489	−0.337387	0.222890
O	2.175451	−0.176213	−0.242639
H	0.808118	−1.248133	0.787358

s-P4 (acetylcyanide + H)

Table 25 Cartesian coordinates in Å of the acetylcyanide structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.435388	0.206437	−0.000013
O	0.875395	1.331535	−0.000061
C	−1.033749	−0.009358	0.000014
N	−2.179015	−0.205280	0.000032
C	1.253779	−1.050580	0.000026
H	1.002871	−1.648213	0.879919
H	1.002857	−1.648277	−0.879819
H	2.311705	−0.797822	0.000008

s-P5 (Formylcyanide + CH_3)

Table 26 Cartesian coordinates in Å of the Formylcyanide structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.692079	0.426205	−0.000021
O	−1.562173	−0.407499	0.000045
C	0.737630	0.069129	−0.000014
N	1.873815	−0.174115	−0.000009
H	−0.892626	1.506792	−0.000090

Table 27 Cartesian coordinates in Å of the CH_3 structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.204697	0.140730	−0.218631
H	0.303637	−0.757915	0.092664
H	0.303657	0.859632	−0.841227
H	−1.221388	0.320469	0.092664

s-P6 (Vinylcyanide + OH)

Table 28 Cartesian coordinates in Å of the vinylcyanide structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.608242	0.671357	0.000006
H	−1.181236	−0.247803	0.000007
C	0.727830	0.662097	0.000002
H	1.269248	−0.274564	0.000000
H	1.298781	1.581579	0.000001
C	−1.365754	1.888472	0.000009
N	−1.997712	2.864467	0.000012

Table 29 Cartesian coordinates in Å of the OH structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
O	−1.121951	0.449697	−0.040988
H	−1.446314	1.365670	−0.040988

s-P7 (Cyanovinylacohol isomer + H)

Table 30 Cartesian coordinates in Å of the Cyanovinylacohol isomer structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	1.186962	0.447476	−0.000000
C	−0.062691	0.933629	0.000000
O	1.443243	−0.876551	0.000001
H	2.392715	−1.026824	−0.000003
H	−0.208611	2.003819	0.000000
C	−1.216174	0.096418	0.000000
N	−2.173932	−0.564025	−0.000000
H	2.038897	1.118445	−0.000000

2.1.2 *anti*-VyA + CN

CN (Cyanide radical)

Table 31 Cartesian coordinates in Å of the cyanide radical structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−1.875383	0.453789	0.017829
N	−0.716421	0.453789	0.017829

C_2H_4O (*anti*-VyA)

Table 32 Cartesian coordinates in Å of the *anti*-Vy structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.035965	0.414901	0.000010
O	−1.132689	−0.296697	0.000001
H	−0.067014	1.495467	0.000038
C	1.225337	−0.181204	−0.000014
H	1.314586	−1.259393	−0.000042
H	2.120535	0.422594	−0.000006
H	−1.874405	0.312722	0.000028

a-Int1

Table 33 Cartesian coordinates in Å of the **a-Int1** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−1.150932	0.386547	−0.375960
O	−1.673440	−0.666779	0.316802
H	−1.273802	0.390953	−1.453333
C	0.096160	0.936729	0.235924
H	−0.041662	1.053629	1.313575
H	0.313950	1.920135	−0.184541
H	−2.377469	−1.073997	−0.196910
C	1.265314	0.068067	0.007300
N	2.169367	−0.628796	−0.203783

a-Int1b

Table 34 Cartesian coordinates in Å of the **a-Int1b** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.607662	0.081245	0.484541
O	1.606201	−0.525769	−0.260327
H	0.752419	0.120428	1.561019
C	−0.106259	1.228763	−0.169707
H	0.170229	1.443178	−1.195284
H	−0.407234	2.069767	0.442932
H	1.605880	−1.469028	−0.065629
C	−0.847937	−0.061981	0.028439
N	−1.815698	−0.780466	−0.084464

a-Int2

Table 35 Cartesian coordinates in Å of the **a-Int2** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.424723	−0.018446	0.383703
O	1.006460	−1.208950	−0.140369
H	0.560788	−0.108137	1.466272
C	1.086852	1.217589	−0.126004
H	2.154941	1.311218	0.005584
H	0.522218	2.012839	−0.587756
H	0.992787	−1.145271	−1.102593
C	−1.033056	0.018850	0.124049
N	−2.170629	0.053585	−0.102315

a-Int3

Table 36 Cartesian coordinates in Å of the **a-Int3** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.988855	−0.451602	0.291772
O	2.181772	0.091644	−0.250676
H	0.700065	−1.384477	−0.203082
C	−0.141240	0.528383	0.246121
H	0.057252	1.572710	0.446049
H	2.046477	0.238001	−1.192277
C	−1.461617	0.120365	0.020576
N	−2.547823	−0.241163	−0.175942
H	1.225660	−0.692625	1.332968

a-Int4

Table 37 Cartesian coordinates in Å of the **a-Int4** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.338179	0.053219	0.000062
O	0.862528	1.306811	0.000292
C	1.325205	−1.052983	0.000045
H	1.968304	−0.991214	0.883150
H	0.816834	−2.015413	−0.000143
H	0.152117	1.959414	0.000287
C	−1.050149	−0.116959	−0.000144
N	−2.208459	−0.235861	−0.000314
H	1.968528	−0.990987	−0.882881

a-Int5

Table 38 Cartesian coordinates in Å of the **a-Int5** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.409848	−0.041316	0.380390
O	1.041703	−1.144416	−0.140658
C	1.125194	1.214977	−0.154543
H	1.065265	1.238867	−1.241852
H	0.635570	2.101157	0.248889
C	−1.038927	0.003264	0.057753
N	−2.171740	0.059832	−0.186926
H	2.168228	1.191981	0.156014
H	0.521602	−0.063452	1.472807

a-TS1

Table 39 Cartesian coordinates in Å of the **a-TS1** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.664408	0.096319	0.485392
O	1.628091	−0.643117	−0.146936
H	0.807188	0.131491	1.555878
C	−0.095778	1.196556	−0.189615
H	0.164647	1.419266	−1.221126
H	−0.351939	2.066418	0.408023
H	1.418229	−0.726769	−1.083829
C	−0.938690	0.000508	0.004124
N	−1.834641	−0.786538	−0.040410

a-TS1b

Table 40 Cartesian coordinates in Å of the **a-TS1b** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.579745	0.065395	0.458799
O	1.577886	−0.582191	−0.265314
H	0.740393	0.115893	1.535460
C	0.020950	1.289451	−0.169491
H	0.192060	1.436633	−1.225814
H	−0.304558	2.112406	0.449097
H	1.542735	−1.523286	−0.062155
C	−0.829581	−0.182495	0.091930
N	−1.904478	−0.640018	−0.123799

a-TS3

Table 41 Cartesian coordinates in Å of the **a-TS3** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	1.250669	0.421444	−0.080454
O	1.448643	−0.922534	−0.134443
H	2.114504	1.008116	0.195654
C	−0.102803	0.996542	0.152658
H	0.500170	1.057870	−0.988633
H	−0.181906	1.956790	0.641123
H	0.610965	−1.384199	0.013819
C	−1.210093	0.115617	0.129903
N	−2.059686	−0.679345	0.077561

a-TS3b

Table 42 Cartesian coordinates in Å of the **a-TS3b** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.255727	0.377936	0.511840
O	1.217745	−1.312316	−0.036073
H	0.515450	0.158045	1.537357
C	1.023432	1.184436	−0.249777
H	0.702847	1.496782	−1.234800
H	1.999153	1.490612	0.098749
H	1.018149	−1.323017	−0.985933
C	−1.099169	0.063911	0.121422
N	−2.190669	−0.166943	−0.188721

a-TS4

Table 43 Cartesian coordinates in Å of the **a-TS4** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.932324	−0.356049	0.095185
O	2.211832	0.008191	−0.097272
H	0.743844	−1.349749	0.485472
C	−0.068127	0.520948	−0.119763
H	0.123225	1.456674	−0.627959
H	−0.169327	1.569052	1.401728
H	2.800709	−0.710917	0.150147
C	−1.424189	0.056413	−0.047216
N	−2.520454	−0.317557	0.002945

a-TS5

Table 44 Cartesian coordinates in Å of the **a-TS5** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.905315	−0.314056	−0.082033
O	−2.182927	0.122117	−0.089299
H	−0.800137	−1.097928	1.581223
C	0.107487	0.562830	0.086076
H	−0.086297	1.593702	0.348374
H	−2.782624	−0.625632	−0.169561
C	1.456715	0.114741	−0.008562
N	2.556411	−0.243981	−0.082571
H	−0.715719	−1.320310	−0.440533

a-TS8

Table 45 Cartesian coordinates in Å of the **a-TS8** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.973209	−0.456428	−0.014424
O	2.161746	−0.170047	−0.093295
H	0.648941	−1.485026	0.189502
C	−0.072654	0.631607	−0.071866
H	0.065333	1.226198	−0.977742
H	0.124238	1.302403	0.776609
H	2.684898	0.765786	0.910022
C	−1.439801	0.121175	−0.002176
N	−2.511700	−0.318159	0.054110

a-TS10

Table 46 Cartesian coordinates in Å of the **a-TS10** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.302171	−0.068947	0.490469
O	0.997951	−1.130198	−0.185764
H	0.385532	−0.151275	1.574392
C	1.221740	0.927431	−0.157514
H	0.828727	1.513614	−0.979728
H	1.998643	1.360990	0.460350
H	1.704876	−0.199318	−0.678716
C	−1.111398	0.022089	0.103609
N	−2.229604	0.112745	−0.193324

a-TS12

Table 47 Cartesian coordinates in Å of the **a-TS12** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.334038	−0.054029	0.133156
O	0.929903	−1.280255	−0.049322
H	0.732929	0.651726	1.118530
C	1.132907	1.179164	−0.041148
H	0.638686	2.112256	−0.261441
H	2.206066	1.076333	−0.087525
H	1.472745	−1.238061	−0.848368
C	−1.091167	0.006170	0.023773
N	−2.249515	0.075763	−0.029666

a-TS13

Table 48 Cartesian coordinates in Å of the **a-TS13** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.404534	0.110560	0.080546
O	0.933802	1.210862	0.154848
C	1.145341	−1.181204	−0.032381
H	2.198169	−1.021530	0.189752
H	0.716415	−1.928851	0.637712
H	1.425798	1.899735	−1.094031
C	−1.063633	0.018064	0.003480
N	−2.214645	−0.085852	−0.057717
H	1.036995	−1.560560	−1.054883

a-TS14

Table 49 Cartesian coordinates in Å of the **a-TS14** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.427525	0.205295	0.055679
O	−0.882098	1.320709	−0.116335
C	−1.236125	−1.069884	−0.062106
H	−1.198752	−1.372550	−1.112793
H	−0.815043	−1.873649	0.540853
C	1.052554	−0.007870	0.004781
N	2.195794	−0.202452	−0.061282
H	−2.268772	−0.870287	0.216498
H	−0.364628	0.202725	1.724963

a-TS15

Table 50 Cartesian coordinates in Å of the **a-TS15** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.310687	0.527182	0.408540
O	−0.868530	1.354743	−0.294369
C	−1.281700	−1.294700	−0.095820
H	−1.035936	−1.322914	−1.148311
H	−0.764334	−1.986617	0.557108
C	1.047279	0.024054	0.078946
N	2.112807	−0.374459	−0.155865
H	−2.289028	−1.004616	0.168934
H	−0.591439	0.351855	1.457777

a-TS16

Table 51 Cartesian coordinates in Å of the **a-TS16** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.436290	0.033779	0.059402
O	0.996474	−1.197203	−0.142723
H	0.329343	−0.013623	1.856427
C	1.172628	1.151842	−0.077762
H	0.693242	2.117949	−0.053825
H	2.248480	1.081821	−0.148338
H	0.412434	−1.880038	0.205614
C	−1.015941	0.089477	−0.006934
N	−2.172698	0.084454	−0.074650

a-P1 (cyanovinylalcohol isomer + H)

Table 52 Cartesian coordinates in Å of the cyanovinylalcohol isomer structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−2.382269	0.945131	−0.000362
H	−2.955911	0.024193	−0.000477
C	−1.042183	0.938093	−0.000079
H	−0.479726	1.862579	0.000035
O	−3.073123	2.105766	−0.000511
H	−4.016875	1.922791	−0.000715
C	−0.329433	−0.294769	0.000078
N	0.266749	−1.294247	0.000210

a-P2 (cyanovinylalcohol isomer + H)

Table 53 Cartesian coordinates in Å of the cyanovinylalcohol isomer structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.443981	0.039262	−0.000001
C	1.198529	1.140439	0.000000
H	2.276862	1.062360	0.000002
O	0.990152	−1.212171	−0.000000
H	0.291376	−1.874294	0.000005
C	−0.994930	0.104485	−0.000001
N	−2.157744	0.098859	0.000001
H	0.729281	2.112173	0.000000

a-P3 (cyanoacetaldehyde + H)

Table 53 Cartesian coordinates in Å of the cyanoacetaldehyde structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−1.345923	0.104809	−0.027948
N	−2.377393	−0.417343	−0.125136
C	−0.023598	0.714489	0.099916
H	0.191721	1.363573	−0.749015
H	−0.003508	1.324207	1.009576
C	1.076489	−0.337387	0.222890
O	2.175451	−0.176213	−0.242639
H	0.808118	−1.248133	0.787358

a-P4 (acetylcyanide + H)

Table 54 Cartesian coordinates in Å of the acetylcyanide structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.435388	0.206437	−0.000013
O	0.875395	1.331535	−0.000061
C	−1.033749	−0.009358	0.000014
N	−2.179015	−0.205280	0.000032
C	1.253779	−1.050580	0.000026
H	1.002871	−1.648213	0.879919
H	1.002857	−1.648277	−0.879819
H	2.311705	−0.797822	0.000008

a-P5 (Formylcyanide + CH_3)

Table 55 Cartesian coordinates in Å of the Formylcyanide structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.692079	0.426205	−0.000021
O	−1.562173	−0.407499	0.000045
C	0.737630	0.069129	−0.000014
N	1.873815	−0.174115	−0.000009
H	−0.892626	1.506792	−0.000090

Table 56 Cartesian coordinates in Å of the CH_3 structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.204697	0.140730	−0.218631
H	0.303637	−0.757915	0.092664
H	0.303657	0.859632	−0.841227
H	−1.221388	0.320469	0.092664

a-P6 (Vinylcyanide + OH)

Table 57 Cartesian coordinates in Å of the vinylcyanide structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.608242	0.671357	0.000006
H	−1.181236	−0.247803	0.000007
C	0.727830	0.662097	0.000002
H	1.269248	−0.274564	0.000000
H	1.298781	1.581579	0.000001
C	−1.365754	1.888472	0.000009
N	−1.997712	2.864467	0.000012

Table 57 Cartesian coordinates in Å of the OH structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
O	−1.121951	0.449697	−0.040988
H	−1.446314	1.365670	−0.040988

a-P7 (Cyanovinylacohol isomer + H)

Table 58 Cartesian coordinates in Å of the Cyanovinylacohol isomer structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−2.378164	1.002522	0.000021
C	−1.037611	1.032446	0.001148
O	−3.122332	2.127217	0.000016
H	−4.056895	1.902113	−0.000884
H	−0.492664	0.099905	0.001093
C	−0.293089	2.247818	0.002424
N	0.338404	3.224906	0.003476
H	−2.907880	0.056270	−0.000931

3 Abstraction reactions

3.1 C attack

3.1.1 *Syn*-VyA + CN

CN (Cyanide radical)

Table 59 Cartesian coordinates in Å of the cyanide radical structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−1.875383	0.453789	0.017829
N	−0.716421	0.453789	0.017829

C_2H_4O (*syn*-VyA)

Table 60 Cartesian coordinates in Å of the *syn*-Vy structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.036309	0.442827	0.000002
O	1.206308	−0.115176	−0.000002
H	0.027835	1.523455	−0.000001
C	−1.199885	−0.207586	0.000001
H	−1.253910	−1.290335	−0.000002
H	−2.123655	0.351690	−0.000006
H	1.116437	−1.074853	0.000005

s-Int1A

Table 61 Cartesian coordinates in Å of the **s-Int1A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−1.223970	0.346877	0.284567
O	−1.480884	−0.913455	−0.162057
H	−2.121561	0.940412	0.387136
C	0.040897	1.030829	−0.153977
H	0.211418	1.921086	0.454209
H	−0.010268	1.353709	−1.203771
H	−0.655988	−1.414046	−0.216449
C	1.190800	0.128598	−0.026067
N	2.045701	−0.651991	0.057004

s-Int1bA

Table 62 Cartesian coordinates in Å of the **s-Int1bA** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.608031	0.077743	0.482179
O	1.603376	−0.532773	−0.264103
H	0.753870	0.115309	1.558569
C	−0.101622	1.228876	−0.170371
H	0.174886	1.443105	−1.195982
H	−0.398541	2.070548	0.443327
H	1.599009	−1.476259	−0.070555
C	−0.848535	−0.058934	0.027189
N	−1.819387	−0.773261	−0.085589

s-TS1A

Table 63 Cartesian coordinates in Å of the **s-TS1A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.130909	0.303384	−0.000883
O	1.315944	−0.042578	−0.331837
H	−0.030529	1.335571	0.304535
C	−0.895449	−0.668380	0.049054
H	−1.045294	−1.330132	−0.792009
H	−1.746029	−0.515125	0.702383
H	1.233527	−1.132287	−0.054210
C	0.470202	−2.218175	0.660811
N	0.170111	−3.185072	1.241917

s-TS1bA

Table 64 Cartesian coordinates in Å of the **s-TS1bA** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.664408	0.096319	0.485392
O	1.628091	−0.643117	−0.146936
H	0.807188	0.131491	1.555878
C	−0.095778	1.196556	−0.189615
H	0.164647	1.419266	−1.221126
H	−0.351939	2.066418	0.408023
H	1.418229	−0.726769	−1.083829
C	−0.938690	0.000508	0.004124
N	−1.834641	−0.786538	−0.040410

s-TS1cA

Table 65 Cartesian coordinates in Å of the **s-TS1cA** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.579745	0.065395	0.458799
O	1.577886	−0.582191	−0.265314
H	0.740393	0.115893	1.535460
C	0.020950	1.289451	−0.169491
H	0.192060	1.436633	−1.225814
H	−0.304558	2.112406	0.449097
H	1.542735	−1.523286	−0.062155
C	−0.829581	−0.182495	0.091930
N	−1.904478	−0.640018	−0.123799

s-TS2A

Table 66 Cartesian coordinates in Å of the **s-TS2A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.069853	0.438801	−0.335670
O	1.243948	−0.188849	−0.225010
H	0.182150	1.503510	−0.820652
C	−1.156256	0.063419	0.037639
H	−1.365697	−0.952973	0.352321
H	−1.967323	0.773367	−0.030503
H	1.239471	−0.770239	0.545814
C	0.145630	2.919826	−0.238803
N	−0.029379	3.519241	0.756247

s-TS3A

Table 67 Cartesian coordinates in Å of the **s-TS3A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.193222	0.476604	0.065339
O	1.045125	0.052372	−0.253161
H	−0.227896	1.551060	0.197349
C	−1.270558	−0.289528	0.269478
H	−1.433198	−1.326715	0.006501
H	−2.257123	0.325340	0.612143
H	1.039488	−0.902539	−0.394914
C	−3.237355	1.228171	0.090881
N	−3.823210	1.946020	−0.613150

s-TS4A

Table 68 Cartesian coordinates in Å of the **s-TS4A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.050678	0.231212	0.039101
O	1.028778	−0.525085	0.209067
H	0.203374	1.279544	−0.105955
C	−1.333780	−0.155453	−0.067900
H	−1.541405	−1.398835	−0.118090
H	−2.208883	0.461544	0.077891
H	0.771430	−1.441110	0.427101
C	−1.162462	−2.597641	0.431178
N	−0.282593	−3.213641	0.896211

s-P1A

Table 69 Cartesian coordinates in Å of the **s-P1A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.059208	0.454794	−0.000002
O	1.125311	−0.131781	0.000001
H	0.025738	1.559621	−0.000000
C	−1.214261	−0.219153	−0.000002
H	−1.236609	−1.300392	−0.000001
H	−2.139004	0.341785	−0.000003

Table 70 Cartesian coordinates in Å of HCN structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.000000	0.000000	−0.628545
N	−0.000000	0.000000	0.528914
H	−0.000000	0.000000	−1.695936

s-P2A

Table 71 Cartesian coordinates in Å of the **s-P2A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.054042	0.069429	0.138012
O	1.052857	−0.543230	−0.283056
C	−1.321854	−0.225732	−0.040456
H	−1.609242	−1.182332	−0.469608
H	−2.091478	0.470355	0.257383
H	1.732745	−0.481923	0.397723

Table 72 Cartesian coordinates in Å of HCN structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.000000	0.000000	−0.628545
N	−0.000000	0.000000	0.528914
H	−0.000000	0.000000	−1.695936

s-P3A

Table 73 Cartesian coordinates in Å of the **s-P3A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.012611	0.418788	−0.000007
O	1.271664	−0.072020	0.000002
H	−0.003559	1.502352	0.000004
C	−1.127518	−0.263480	−0.000002
H	−1.501967	−1.271953	0.000002
H	1.234468	−1.035354	0.000004

Table 74 Cartesian coordinates in Å of HCN structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.000000	0.000000	−0.628545
N	−0.000000	0.000000	0.528914
H	−0.000000	0.000000	−1.695936

s-P4A

Table 75 Cartesian coordinates in Å of the **s-P4A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.004196	0.478756	−0.000000
O	1.213723	−0.136214	0.000004
H	0.104127	1.561250	−0.000002
C	−1.179311	−0.095034	−0.000003
H	−2.211761	0.201486	−0.000001
H	1.068150	−1.089887	0.000002

Table 76 Cartesian coordinates in Å of HCN structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.000000	0.000000	−0.628545
N	−0.000000	0.000000	0.528914
H	−0.000000	0.000000	−1.695936

3.1.2 *Anti*-VyA + CN

CN (Cyanide radical)

Table 77 Cartesian coordinates in Å of the cyanide radical structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−1.875383	0.453789	0.017829
N	−0.716421	0.453789	0.017829

C_2H_4O (*anti*-VyA)

Table 78 Cartesian coordinates in Å of the *anti*-Vy structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.035965	0.414901	0.000010
O	−1.132689	−0.296697	0.000001
H	−0.067014	1.495467	0.000038
C	1.225337	−0.181204	−0.000014
H	1.314586	−1.259393	−0.000042
H	2.120535	0.422594	−0.000006
H	−1.874405	0.312722	0.000028

a-Int1A

Table 79 Cartesian coordinates in Å of the **a-Int1A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−1.150932	0.386547	−0.375960
O	−1.673440	−0.666779	0.316802
H	−1.273802	0.390953	−1.453333
C	0.096160	0.936729	0.235924
H	−0.041662	1.053629	1.313575
H	0.313950	1.920135	−0.184541
H	−2.377469	−1.073997	−0.196910
C	1.265314	0.068067	0.007300
N	2.169367	−0.628796	−0.203783

a-Int1bA

Table 80 Cartesian coordinates in Å of the **a-Int1bA** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.607662	0.081245	0.484541
O	1.606201	−0.525769	−0.260327
H	0.752419	0.120428	1.561019
C	−0.106259	1.228763	−0.169707
H	0.170229	1.443178	−1.195284
H	−0.407234	2.069767	0.442932
H	1.605880	−1.469028	−0.065629
C	−0.847937	−0.061981	0.028439
N	−1.815698	−0.780466	−0.084464

a-TS1A

Table 81 Cartesian coordinates in Å of the **a-TS1A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	2.159762	0.075152	0.102454
H	2.810200	0.866839	−0.238828
H	2.574629	−0.837506	0.507176
C	0.750901	0.229138	0.021189
H	0.283716	1.133043	−0.380200
O	−0.011734	−0.683017	0.414278
H	−1.089903	−0.313440	0.241563
C	−2.164168	0.628275	−0.182312
N	−2.863175	−0.244210	0.193974

a-TS1bA

Table 82 Cartesian coordinates in Å of the **a-TS1bA** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.664408	0.096319	0.485392
O	1.628091	−0.643117	−0.146936
H	0.807188	0.131491	1.555878
C	−0.095778	1.196556	−0.189615
H	0.164647	1.419266	−1.221126
H	−0.351939	2.066418	0.408023
H	1.418229	−0.726769	−1.083829
C	−0.938690	0.000508	0.004124
N	−1.834641	−0.786538	−0.040410

a-TS1cA

Table 83 Cartesian coordinates in Å of the **a-TS1cA** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.579745	0.065395	0.458799
O	1.577886	−0.582191	−0.265314
H	0.740393	0.115893	1.535460
C	0.020950	1.289451	−0.169491
H	0.192060	1.436633	−1.225814
H	−0.304558	2.112406	0.449097
H	1.542735	−1.523286	−0.062155
C	−0.829581	−0.182495	0.091930
N	−1.904478	−0.640018	−0.123799

a-TS2A

Table 84 Cartesian coordinates in Å of the **a-TS2A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.125935	0.526500	−0.110469
O	−1.205310	−0.147513	0.303887
H	−0.316904	1.547658	−0.625836
C	1.141653	0.163914	0.093029
H	1.387740	−0.832150	0.440043
H	1.930984	0.863823	−0.137811
H	−1.974381	0.099030	−0.223160
C	−0.219055	3.054204	−0.132064
N	0.128120	3.731933	0.763958

a-TS3A

Table 85 Cartesian coordinates in Å of the **a-TS3A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.209844	0.452587	−0.038680
O	−0.992465	−0.091813	0.246408
H	0.239994	1.523590	−0.214966
C	1.317373	−0.286438	−0.143926
H	1.492310	−1.303187	0.178921
H	2.305615	0.361010	−0.450970
H	−1.680272	0.575355	0.156657
C	3.146720	1.391425	0.037578
N	3.532066	2.298236	0.657416

a-TS4A

Table 86 Cartesian coordinates in Å of the **a-TS4A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.046295	0.326152	0.053876
O	−1.094324	−0.375407	−0.111901
H	−0.053940	1.382511	0.294616
C	1.253619	−0.211020	−0.121272
H	1.306860	−1.356155	−0.447955
H	2.191418	0.250450	0.147217
H	−1.854055	0.206649	−0.020874
C	1.265516	−2.733061	0.073106
N	1.232151	−3.663263	0.768092

a-P1A

Table 87 Cartesian coordinates in Å of the **a-P1A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.058371	0.399573	0.000009
O	−1.088306	−0.248410	0.000001
H	−0.089641	1.504464	0.000040
C	1.252370	−0.198665	−0.000015
H	1.337980	−1.276741	−0.000042
H	2.142688	0.415448	−0.000007

Table 88 Cartesian coordinates in Å of HCN structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.000000	0.000000	−0.628545
N	−0.000000	0.000000	0.528914
H	−0.000000	0.000000	−1.695936

a-P2A

Table 89 Cartesian coordinates in Å of the **a-P2A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.026173	0.349130	−0.098557
O	−1.171265	−0.215784	−0.256321
C	1.222768	−0.184205	0.001602
H	1.338199	−1.257954	0.126447
H	2.102483	0.441336	−0.017486
H	−1.829030	0.280399	0.244292

Table 90 Cartesian coordinates in Å of HCN structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.000000	0.000000	−0.628545
N	−0.000000	0.000000	0.528914
H	−0.000000	0.000000	−1.695936

a-P3A

Table 91 Cartesian coordinates in Å of the **a-P3A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.005398	0.375009	0.000011
O	−1.226214	−0.262981	0.000008
H	−0.043998	1.461208	0.000038
C	1.140067	−0.249715	−0.000017
H	1.556621	−1.240624	−0.000045
H	−1.919299	0.402899	0.000025

Table 92 Cartesian coordinates in Å of HCN structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.000000	0.000000	−0.628545
N	−0.000000	0.000000	0.528914
H	−0.000000	0.000000	−1.695936

a-P4A

Table 93 Cartesian coordinates in Å of the **a-P4A** structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	0.013981	0.437970	0.000012
O	−1.132688	−0.309220	0.000003
H	−0.123402	1.520677	0.000040
C	1.215637	−0.071824	−0.000012
H	2.221555	0.305237	−0.000011
H	−1.887354	0.284943	0.000024

Table 94 Cartesian coordinates in Å of HCN structure optimized at rev-DSDPBEP86-GD3BJ/jun-cc-pVTZ level of theory.

Atom	X	Y	Z
C	−0.000000	0.000000	−0.628545
N	−0.000000	0.000000	0.528914
H	−0.000000	0.000000	−1.695936

4 Energy tables

4.1 Addition reactions

anti-VyA + CN			*syn*-VyA + CN		
Species	**rDSD**	**junChS-F12**	**Species**	**rDSD**	**junChS-F12**
A+B	0.0	0.0	**A+B**	0.0	0.0
a-Int1	-247.9	-230.3	**s-Int1**	-242.9	-225.9
a-Int1b	-117.7	-115.1	**s-Int1b**	-117.7	-109.6
a-Int2	-209.7	-197.9	**s-Int2**	-209.7	-192.6
a-Int3	-249.3	-234.7	**s-Int3**	-246.4	-231.3
a-Int4	-284.1	-273.2	**s-Int4**	-284.1	-267.9
a-Int5	-187.1	-175.1	**s-Int5**	-187.1	-169.8
a-TS1	-112.7	-114.1	**s-TS1**	-112.7	-101.8
a-TS1b	-104.1	-99.6	**s-TS1b**	-104.1	-94.4
a-TS3	-77.1	-66.2	**s-TS3**	-77.1	-60.9
a-TS3b	-92.0	-92.4	**s-TS3b**	-92.0	-87.1
a-TS4	-91.4	-77.2	**s-TS4**	-87.2	-73.1
a-TS5	-90.7	-76.9	**s-TS5**	-84.5	-71.1
a-TS8	-85.5	-73.4	**s-TS8**	-85.5	-68.1
a-TS10	-73.3	-63.8	**s-TS10**	-73.3	-58.5
a-TS12	-63.2	52.9	**s-TS12**	-63.2	-47.6
a-TS13	-96.3	-81.4	**s-TS13**	-96.3	-76.1
a-TS14	-96.4	-82.6	**s-TS14**	-96.4	-77.4
a-TS15	-121.3	-106.9	**s-TS15**	-121.3	-101.6
a-TS16	-58.4	-51.9	**s-TS16**	-56.4	-46.6
a-P1	-115.5	-98.6	**s-P1**	-116.7	-94.3
a-P2	-100.4	-85.1	**s-P2**	-100.4	-79.8
a-P3	-134.6	-114.9	**s-P3**	-134.6	-109.6
a-P4	-140.1	-119.5	**s-P4**	-140.1	-114.2
a-P5	-131.6	-116.0	**s-P5**	-131.6	-110.7
a-P6	-112.0	-101.5	**s-P6**	-112.0	-96.2
a-P7	-126.0	-109.4	**s-P7**	-125.9	-104.1

Table 95 Anharmonic Zero-point Corrected Energies (in kJ mol^{-1}) Relative to the Dissociation Limit for All the Species Involved in the *syn*-VyA + CN and *anti*-VyA + CN Addition Reactions Computed Using the Two Different Levels of Theory Discussed in Section 2.

4.2 Abstraction reactions

4.2.1 C attack

anti-VyA + CN			*syn*-VyA + CN		
Species	**rDSD**	**junChS-F12**	**Species**	**rDSD**	**junChS-F12**
A+B	0.0	0.0	**A+B**	0.0	0.0
a-Int1A	-247.9	-230.3	**s-Int1A**	-242.9	-225.9
a-Int1bA	-117.7	-115.1	**s-Int1bA**	-117.7	-109.6
a-TS1A	-42.4	-23.2	**s-TS1A**	-64.7	-44.2
a-TS1bA	-112.7	-114.1	**s-TS1bA**	-112.7	-101.8
a-TS1cA	-104.1	-99.6	**s-TS1cA**	-104.1	-94.4
a-TS2A	-6.3	10.6	**s-TS2A**	5.0	21.0
a-TS3A	-6.5	6.9	**s-TS3A**	-5.3	8.5
a-TS4A	-4.9	7.7	**s-TS4A**	-16.9	-3.2
a-P1A	-192.2	-177.9	**s-P1A**	-187.6	-173.1
a-P2A	-91.0	-79.6	**s-P2A**	-86.4	-74.8
a-P3A	-61.6	-58.2	**s-P3A**	-57.0	-53.4
a-P4A	-63.5	-63.8	**s-P4A**	-58.9	-59.0

Table 96 Anharmonic Zero-point Corrected Energies (in kJ mol^{-1}) Relative to the Dissociation Limit for All the Species Involved in the *syn*-VyA + CN and *anti*-VyA + CN Abstraction Reactions Computed Using the Two Different Levels of Theory Discussed in Section 2.

5 MESS input files

5.1 *Syn*-VyA + CN

```
!************************************************
!               GLOBAL SECTION
!************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

TemperatureList[K]                      30 40 50 60 70 80 90 100 110 120
                                        130 140 150 160 170 180 190 200
                                        210 220 230 240 250 260 270 280
                                        290 300 310 320 330 340 350 360
                                        370 380 390 400 410 420 430 440
                                        450 460 470 480 490 500 510 520
                                        530 540 550 560 570 580 590 600
PressureList[atm]                       1.e-8 1
EnergyStepOverTemperature               .2
ExcessEnergyOverTemperature             30
ModelEnergyLimit[kcal/mol]              400
CalculationMethod                       low-eigenvalue
WellCutoff                              20
ChemicalEigenvalueMax                   0.2
ReductionMethod                         projection
AtomDistanceMin[bohr]                  1.3
RateOutput                              rate.out


!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!************************************************
!               MODEL SECTION
!************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!


Model

  EnergyRelaxation
    Exponential
       Factor[1/cm]                     260
       Power                            0.85
       ExponentCutoff                   15
End

CollisionFrequency
    LennardJones
       Epsilons[K]                       127.697  1280.940
       Sigmas[angstrom]                  3.462    4.495
       Masses[amu]                       39.948 70.07098
   End

!************************************************
!
!************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!************************************************
!  REACTANT syn-Vy + CN
```

```
!************************************************
 Bimolecular REACS
 Fragment C2H4O
 RRHO
 Geometry[angstrom]                7
 C     -0.036309     0.442827     0.000002
 O      1.206308    -0.115176    -0.000002
 H      0.027835     1.523455    -0.000001
 C     -1.199885    -0.207586     0.000001
 H     -1.253910    -1.290335    -0.000002
 H     -2.123655     0.351690    -0.000006
 H      1.116437    -1.074853     0.000005
Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]       15
  447.1190 488.0154 716.3502
  829.9799 962.9976 999.9229
  1123.4916 1331.1630 1356.5408
  1456.4521 1702.4021 3163.9015
  3216.3548 3269.8330 3817.0327
  ZeroEnergy[kJ/mol]              0.
  ElectronicLevels[1/cm]                      1
   0            1
 !**********************************
 End
!*********
 Fragment CN
 RRHO
 Geometry[angstrom]                2
 C     -1.875383     0.453789     0.017829
 N     -0.716421     0.453789     0.017829
Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]   1
  2411.1619
  ZeroEnergy[kJ/mol]              0.
  ElectronicLevels[1/cm]                      1
   0            2
 !**********************************
 End
!*********
GroundEnergy[kJ/mol] 0.0
End
!************************************************
!  PRODUCT P1
!************************************************
 Bimolecular P1
 Fragment C3H3NO
 RRHO
 Geometry[angstrom]                8
 C     -0.928205    -0.382036     0.000000
 H     -0.737944    -1.447545     0.000000
 C      0.066381     0.520301     0.000000
 H     -0.130291     1.586302     0.000000
 O     -2.245078    -0.107506     0.000000
```

```
 H    -2.383240     0.847574    -0.000000
 C     1.427541     0.100522     0.000000
 N     2.545400    -0.222715    -0.000000
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    18
  177.8672 191.9231 446.1290
  480.9153 525.8791 554.5641
  807.4403 995.6009 1033.3436
  1155.9231 1269.5349 1341.9119
  1398.5694 1702.1272 2262.1464
  3192.1499 3227.9142 3803.9608
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                     1
   0.0000000000000000        1.0000000000000000
    !**********************************
 End
!*********
 Fragment HYDROGEN
  Atom
  Name H
  ElectronicLevels[1/cm]       1
   0       2
   !***********************************
 End
!*********
GroundEnergy[kJ/mol] -94.30
End
!************************************************
!  PRODUCT P2
!************************************************
 Bimolecular P2
 Fragment C3H3NO
 RRHO
 Geometry[angstrom]               8
 C     0.443981     0.039262    -0.000001
 C     1.198529     1.140439     0.000000
 H     2.276862     1.062360     0.000002
 O     0.990152    -1.212171    -0.000000
 H     0.291376    -1.874294     0.000005
 C    -0.994930     0.104485    -0.000001
 N    -2.157744     0.098859     0.000001
 H     0.729281     2.112173     0.000000
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    18
  193.3575 232.2772 291.3889
  422.2905 608.0666 637.7575
  739.3691 797.2002 886.2303
  985.2469 1240.7954 1342.9461
  1440.1943 1714.9378 2258.4905
  3190.6084 3296.5683 3843.1869
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                     1
   0.0000000000000000        1.0000000000000000
```

```
    !**********************************
 End
!*********
 Fragment HYDROGEN
  Atom
  Name H
  ElectronicLevels[1/cm]       1
   0       2
   !**********************************
 End
!*********
GroundEnergy[kJ/mol] -79.80
End
!************************************************
!  PRODUCT P3
!************************************************
 Bimolecular P3
 Fragment C3H3NO
 RRHO
 Geometry[angstrom]               8
 C    -1.345923     0.104809    -0.027948
 N    -2.377393    -0.417343    -0.125136
 C    -0.023598     0.714489     0.099916
 H     0.191721     1.363573    -0.749015
 H    -0.003508     1.324207     1.009576
 C     1.076489    -0.337387     0.222890
 O     2.175451    -0.176213    -0.242639
 H     0.808118    -1.248133     0.787358
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    18
  61.1798 181.1152 351.3555
  469.1521 521.0854 737.8674
  964.6614 1046.0583 1050.0161
  1227.9169 1297.3395 1419.0734
  1451.8066 1794.2927 2284.8892
  2973.3366 3061.7878 3137.0962
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        1.0000000000000000
    !**********************************
 End
!*********
 Fragment HYDROGEN
  Atom
  Name H
  ElectronicLevels[1/cm]       1
   0       2
   !**********************************
 End
!*********
GroundEnergy[kJ/mol] -109.60
End
!************************************************
!  PRODUCT P4
!************************************************
```

```
 Bimolecular P4
 Fragment C3H3NO
 RRHO
 Geometry[angstrom]                8
 C      0.435388     0.206437    -0.000013
 O      0.875395     1.331535    -0.000061
 C     -1.033749    -0.009358     0.000014
 N     -2.179015    -0.205280     0.000032
 C      1.253779    -1.050580     0.000026
 H      1.002871    -1.648213     0.879919
 H      1.002857    -1.648277    -0.879819
 H      2.311705    -0.797822     0.000008
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    18
  136.5165 177.0018 250.3718
  433.1108 589.6386 595.9424
  724.1801 993.0990 1050.8204
  1209.4700 1405.3542 1472.7222
  1480.6838 1770.4367 2246.8223
  3053.6406 3124.0572 3176.6486
  ZeroEnergy[kJ/mol]              0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        1.0000000000000000
    !***********************************
 End
!*********
 Fragment HYDROGEN
  Atom
  Name H
  ElectronicLevels[1/cm]       1
   0       2
   !***********************************
 End
!*********
GroundEnergy[kJ/mol] -114.20
End
!************************************************
!  PRODUCT P5
!************************************************
 Bimolecular P5
 Fragment C2HNO
 RRHO
 Geometry[angstrom]                5
 C     -0.692079     0.426205    -0.000021
 O     -1.562173    -0.407499     0.000045
 C      0.737630     0.069129    -0.000014
 N      1.873815    -0.174115    -0.000009
 H     -0.892626     1.506792    -0.000090
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    9
  224.6826 297.9226 616.1239
  927.4680 998.9194 1413.0009
  1751.8461 2250.0589 3033.9889
```

```
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        1.0000000000000000
    !**********************************
 End
!*********
  Fragment CH3
  RRHO
  Geometry[angstrom]               4
 C    -0.204697     0.140730    -0.218631
 H     0.303637    -0.757915     0.092664
 H     0.303657     0.859632    -0.841227
 H    -1.221388     0.320469     0.092664
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    6
  488.3360 1430.3272 1430.3273
  3136.9147 3319.3943 3319.3943
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]       1
   0       2
    !***********************************
 End
!*********
GroundEnergy[kJ/mol] -110.70
End
!************************************************
!  PRODUCT P6
!************************************************
 Bimolecular P6
 Fragment C3H3N
 RRHO
 Geometry[angstrom]               7
 C    -0.608242     0.671357     0.000006
 H    -1.181236    -0.247803     0.000007
 C     0.727830     0.662097     0.000002
 H     1.269248    -0.274564     0.000000
 H     1.298781     1.581579     0.000001
 C    -1.365754     1.888472     0.000009
 N    -1.997712     2.864467     0.000012
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    15
  230.6762 340.8485 566.7814
  702.0030 880.3037 987.8886
  1010.4583 1111.1755 1322.6420
  1453.7345 1675.5742 2263.3312
  3172.0516 3204.5565 3270.4973
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        1.0000000000000000
    !**********************************
 End
!*********
  Fragment HO
```

```
  RRHO
  Geometry[angstrom]                2
 O     -1.121951      0.449697     -0.040988
 H     -1.446314      1.365670     -0.040988
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]     1
  3757.1215
  ZeroEnergy[kJ/mol]              0.
  ElectronicLevels[1/cm]        1
   0       2
    !***********************************
 End
!*********
GroundEnergy[kJ/mol] -96.20
End
!************************************************
!  PRODUCT P7
!************************************************
 Bimolecular P7
 Fragment C3H3NO
 RRHO
 Geometry[angstrom]                8
 C      1.186962      0.447476     -0.000000
 C     -0.062691      0.933629      0.000000
 O      1.443243     -0.876551      0.000001
 H      2.392715     -1.026824     -0.000003
 H     -0.208611      2.003819      0.000000
 C     -1.216174      0.096418      0.000000
 N     -2.173932     -0.564025     -0.000000
 H      2.038897      1.118445     -0.000000
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    18
  149.3755 270.1390 371.8154
  405.5380 590.2572 728.6013
  744.5695 949.8776 952.8482
  1118.2506 1256.9964 1305.2108
  1437.4753 1726.3904 2260.3805
  3191.4026 3239.6076 3862.2591
  ZeroEnergy[kJ/mol]              0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        1.0000000000000000
    !***********************************
 End
!*********
 Fragment HYDROGEN
  Atom
  Name H
  ElectronicLevels[1/cm]        1
   0       2
    !***********************************
 End
!*********
GroundEnergy[kJ/mol] -104.1
```

```
End
!************************************************
!  INT1
!************************************************
 Well INT1
 Species
 RRHO     ! well
 Geometry[angstrom]               9
 C    -1.223970     0.346877     0.284567
 O    -1.480884    -0.913455    -0.162057
 H    -2.121561     0.940412     0.387136
 C     0.040897     1.030829    -0.153977
 H     0.211418     1.921086     0.454209
 H    -0.010268     1.353709    -1.203771
 H    -0.655988    -1.414046    -0.216449
 C     1.190800     0.128598    -0.026067
 N     2.045701    -0.651991     0.057004
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]            21
  104.8434 195.4863 359.0316
  396.3923 430.4077 571.8361
  704.2136 878.3949 930.9778
  1008.3447 1190.8113 1219.3940
  1318.5625 1356.7911 1438.6752
  1464.7128 2280.3431 2997.9781
  3110.1984 3224.7627 3776.2105
  ZeroEnergy[kJ/mol]      -225.90
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        2.0000000000000000
 End
 End
!************************************************
!  INT1b
!************************************************
 Well INT1b
 Species
 RRHO     ! well
 Geometry[angstrom]               9
 C     0.608031     0.077743     0.482179
 O     1.603376    -0.532773    -0.264103
 H     0.753870     0.115309     1.558569
 C    -0.101622     1.228876    -0.170371
 H     0.174886     1.443105    -1.195982
 H    -0.398541     2.070548     0.443327
 H     1.599009    -1.476259    -0.070555
 C    -0.848535    -0.058934     0.027189
 N    -1.819387    -0.773261    -0.085589
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]            21
  192.9948 303.4593 341.8400
  407.9965 480.9881 632.8981
  744.7721 853.2036 947.4843
  1046.2638 1060.5682 1126.4775
```

```
  1202.6147 1291.1035 1403.3887
  1450.6253 1912.9150 3140.8455
  3143.1163 3245.5710 3827.3056
  ZeroEnergy[kJ/mol]      -109.60
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        2.0000000000000000
 End
 End
!************************************************
!  INT2
!************************************************
 Well INT2
 Species
 RRHO     ! well
 Geometry[angstrom]               9
 C     0.424723    -0.018446     0.383703
 O     1.006460    -1.208950    -0.140369
 H     0.560788    -0.108137     1.466272
 C     1.086852     1.217589    -0.126004
 H     2.154941     1.311218     0.005584
 H     0.522218     2.012839    -0.587756
 H     0.992787    -1.145271    -1.102593
 C    -1.033056     0.018850     0.124049
 N    -2.170629     0.053585    -0.102315
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]            21
  65.8557 190.8567 232.0591
  334.9546 393.3755 509.3741
  574.5730 613.0193 807.2125
  976.1030 1089.5257 1125.7179
  1237.7492 1346.9905 1413.0694
  1469.2960 2274.6364 3057.1023
  3184.8072 3308.6257 3809.8375
  ZeroEnergy[kJ/mol]      -192.60
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        2.0000000000000000
 End
 End
!************************************************
!  INT3
!************************************************
 Well INT3
 Species
 RRHO     ! well
 Geometry[angstrom]               9
 C     0.988855    -0.451602     0.291772
 O     2.181772     0.091644    -0.250676
 H     0.700065    -1.384477    -0.203082
 C    -0.141240     0.528383     0.246121
 H     0.057252     1.572710     0.446049
 H     2.046477     0.238001    -1.192277
 C    -1.461617     0.120365     0.020576
 N    -2.547823    -0.241163    -0.175942
 H     1.225660    -0.692625     1.332968
  Core  RigidRotor
```

```
 SymmetryFactor    1.0000000000000000
 End
    Frequencies[1/cm]            21
 47.0339 185.5126 325.0330
 394.7722 428.4037544.6996
 577.9890 887.5487 1041.8618
 1071.4663 1120.2467 1195.5659
 1320.2677 1398.8290 1428.7017
 1498.8184 2316.6123 3036.8405
 3078.0715 3225.4018 3834.6120
 ZeroEnergy[kJ/mol]      -231.30
 ElectronicLevels[1/cm]                      1
  0.0000000000000000        2.0000000000000000
End
End
!***************************************************
!  INT4
!***************************************************
Well INT4
Species
RRHO     ! well
Geometry[angstrom]               9
C     0.338179     0.053219     0.000062
O     0.862528     1.306811     0.000292
C     1.325205    -1.052983     0.000045
H     1.968304    -0.991214     0.883150
H     0.816834    -2.015413    -0.000143
H     0.152117     1.959414     0.000287
C    -1.050149    -0.116959    -0.000144
N    -2.208459    -0.235861    -0.000314
H     1.968528    -0.990987    -0.882881
 Core  RigidRotor
 SymmetryFactor    1.0000000000000000
 End
    Frequencies[1/cm]            21
 90.6477 190.0395 238.3457
 385.8546 404.4841 461.3178
 621.5631 749.7738 1015.0283
 1023.8833 1172.6828 1366.3166
 1411.4686 1441.0116 1478.6647
 1511.7408 2329.9872 3034.6289
 3090.0035 3159.0180 3814.6683
 ZeroEnergy[kJ/mol]      -267.90
 ElectronicLevels[1/cm]                      1
  0.0000000000000000        2.0000000000000000
End
End
!***************************************************
!  INT5
!***************************************************
Well INT5
Species
RRHO     ! well
Geometry[angstrom]               9
C     0.409848    -0.041316     0.380390
O     1.041703    -1.144416    -0.140658
C     1.125194     1.214977    -0.154543
```

```
 H     1.065265     1.238867    -1.241852
 H     0.635570     2.101157     0.248889
 C    -1.038927     0.003264     0.057753
 N    -2.171740     0.059832    -0.186926
 H     2.168228     1.191981     0.156014
 H     0.521602    -0.063452     1.472807
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]            21
  185.9006 214.4629 245.7042
  293.8295 505.1179 579.8116
  800.6449 894.3748 985.6645
  1041.5556 1122.4717 1232.4704
  1350.7839 1406.0258 1493.4699
  1510.1447 2273.0772 3017.1289
  3071.1608 3161.0452 3171.1542
  ZeroEnergy[kJ/mol]      -169.80
  ElectronicLevels[1/cm]                     1
   0.0000000000000000        2.0000000000000000
 End
 End
!************************************************
!  BARRIERLESS ENTRANCE CHANNEL - PHASE SPACE THEORY
!************************************************
 Barrier B0 REACS INT1
   RRHO
     Stoichiometry  C3H4N1O1
     Core PhaseSpaceTheory
       FragmentGeometry[angstrom]              7
 C    -0.036309     0.442827     0.000002
 O     1.206308    -0.115176    -0.000002
 H     0.027835     1.523455    -0.000001
 C    -1.199885    -0.207586     0.000001
 H    -1.253910    -1.290335    -0.000002
 H    -2.123655     0.351690    -0.000006
 H     1.116437    -1.074853     0.000005
       FragmentGeometry[angstrom]              2
 C    -1.875383     0.453789     0.017829
 N    -0.716421     0.453789     0.017829
SymmetryFactor     1.0000000000000000
           PotentialPrefactor[au]       64.087
           PotentialPowerExponent  6
      End
     Frequencies[1/cm]            16
  447.1190 488.0154 716.3502
  829.9799 962.9976 999.9229
  1123.4916 1331.1630 1356.5408
  1456.4521 1702.4021 3163.9015
  3216.3548 3269.8330 3817.0327
  2411.1619
  ZeroEnergy[kJ/mol]            0.
  ElectronicLevels[1/cm]                    1
   0.0000000000000000        2.0000000000000000
    End
 !**********************************
  Barrier TS1 INT1 INT1b
```

```
 RRHO
  Geometry[angstrom]            9
C     0.667077     0.096591     0.485498
O     1.634643    -0.636635    -0.148131
H     0.807100     0.126835     1.556499
C    -0.094898     1.197815    -0.185872
H     0.167373     1.426518    -1.215603
H    -0.355272     2.063858     0.415481
H     1.427359    -0.716241    -1.085950
C    -0.934516    -0.001828    -0.000229
N    -1.827872    -0.791445    -0.050937
 Core  RigidRotor
   SymmetryFactor   1
 End
 Rotor Hindered
 Group 7
 Axis 1 2
 Potential[kJ/mol] 24
 0.0
 0.384531131041655
 1.47030644085475
 2.89502436536483
 4.31435212655795
 5.6060688479987
 6.79707940421117
 7.8849866795811
 8.74069374275182
 9.06711207726815
 8.43506397539111
 6.49114222014795
 3.19850930340067
 -0.960534345751633
 -5.07495242028298
 -8.14490401874958
 -9.42151925209061
 -8.6796217644428
 -6.31733649378974
 -3.27931161061933
 -0.698192063120729
 0.661604741482321
 0.780898464158717
 0.297642969226459
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 577.5630
   WellDepth[kJ/mol]    124.10
   WellDepth[kJ/mol]    7.80
   End
   Frequencies[1/cm] 20
 138.0329 249.1384 337.9022
 415.4476 478.4118 783.9889
 849.4804 941.7737 1007.2288
 1077.2953 1117.7864 1207.2879
 1324.7120 1423.5397 1453.1612
 2030.3371 3108.0357 3199.1384
 3229.6599 3820.9414
   ZeroEnergy[kJ/mol]        -101.80
```

```
   ElectronicLevels[1/cm]                    1
      0        2
End
  !**********************************
 Barrier TS1b INT1b INT2
 RRHO
  Geometry[angstrom]            9
C     0.567096     0.035035     0.461466
O     1.512286    -0.722091    -0.229405
H     0.712619     0.082565     1.540513
C     0.009785     1.273776    -0.165612
H     0.165385     1.425643    -1.224305
H    -0.316229     2.095358     0.455608
H     2.297633    -0.175153    -0.345094
C    -0.830667    -0.191724     0.084663
N    -1.919283    -0.622029    -0.124941
  Core  RigidRotor
   SymmetryFactor   1
 End
 Rotor Hindered
 Group 7
 Axis 1 2
 Potential[kJ/mol] 24
 0.0
 0.489270730274633
 1.89197199562412
 3.70901043041916
 5.04851037719963
 5.00146143429436
 3.18676419744718
 0.033827921400906
 -3.41981157783085
 -6.04393324540262
 -7.09080733819441
 -6.46648009661861
 -4.74323869406182
 -2.8628469386589
 -1.66592431936764
 -1.39529596020829
 -1.59447630297682
 -1.55602531634445
 -0.874531418291028
 0.290695245081544
 1.33462459496117
 1.65246256235773
 1.16385733293389
 0.37928981933274
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 677.9480
   WellDepth[kJ/mol]    15.20
   WellDepth[kJ/mol]    98.20
   End
   Frequencies[1/cm] 20
211.4278 226.3736 351.7120
406.1711 492.1999 745.8929
824.8348 873.6945 894.5697
```

```
1080.2098 1167.7307 1205.7098
1306.4266 1393.4610 1449.8594
2042.6957 3107.2677 3170.6329
3294.3832 3813.4662
   ZeroEnergy[kJ/mol]       -94.40
   ElectronicLevels[1/cm]                     1
      0        2
End
  !***********************************
 Barrier TS3 INT1 INT3
 RRHO
  Geometry[angstrom]            9
C     1.250669     0.421444    -0.080454
O     1.448643    -0.922534    -0.134443
H     2.114504     1.008116     0.195654
C    -0.102803     0.996542     0.152658
H     0.500170     1.057870    -0.988633
H    -0.181906     1.956790     0.641123
H     0.610965    -1.384199     0.013819
C    -1.210093     0.115617     0.129903
N    -2.059686    -0.679345     0.077561
  Core MultiRotor
   SymmetryFactor  1.0
   InterpolationEnergyMax[kJ/mol]  1000
   PotentialEnergySurface[kJ/mol] ./TS3.dat
   InternalRotation
Group 7
Axis 1 2
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   InternalRotation
Group 7 9
Axis 4 1
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 1924.2687
   WellDepth[kJ/mol]   165.00
   WellDepth[kJ/mol]   170.40
   End
   Frequencies[1/cm] 20
 130.8542 206.6971 331.0802
 412.6942 432.8810 657.4672
 683.1535 813.3618 895.1560
 1076.6411 1193.8244 1273.1801
 1327.2376 1359.2747 1433.7286
 2145.0885 2327.6981 3224.0019
 3234.3662 3749.8659
   ZeroEnergy[kJ/mol]        -60.90
   ElectronicLevels[1/cm]                     1
      0        2
End
```

```
  !**********************************
 Barrier TS3b INT2 P6
 RRHO
  Geometry[angstrom]            9
C     0.255727     0.377936     0.511840
O     1.217745    -1.312316    -0.036073
H     0.515450     0.158045     1.537357
C     1.023432     1.184436    -0.249777
H     0.702847     1.496782    -1.234800
H     1.999153     1.490612     0.098749
H     1.018149    -1.323017    -0.985933
C    -1.099169     0.063911     0.121422
N    -2.190669    -0.166943    -0.188721
  Core MultiRotor
   SymmetryFactor  1.0
   InterpolationEnergyMax[kJ/mol]  1000
   PotentialEnergySurface[kJ/mol] ./TS3b.dat
   InternalRotation
Group  7
Axis 1 2
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   InternalRotation
Group  6 8
Axis  4 1
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 552.4366
   WellDepth[kJ/mol]    105.5
   WellDepth[kJ/mol]    9.10
   End
   Frequencies[1/cm] 20
 144.9891 171.3810 223.1567
 281.2298 429.4659 567.6507
 670.0482 796.9721 875.3571
 974.7342 1047.7554 1114.9621
 1310.1136 1454.4357 1640.7606
 2416.6629 3180.9562 3233.0109
 3288.9018 3757.0446
   ZeroEnergy[kJ/mol]        -87.10
   ElectronicLevels[1/cm]                      1
      0        2
End
  !**********************************
 Barrier TS4 INT1 P1
 RRHO
  Geometry[angstrom]            9
C     0.928335    -0.404711     0.085427
O     2.237659    -0.159495    -0.041233
H     0.729286    -1.408639     0.435211
C    -0.058345     0.500858    -0.104044
```

```
H     0.137177     1.445670    -0.597098
H    -0.106689     1.512462     1.426851
H     2.381454     0.753701    -0.319982
C    -1.424697     0.063416    -0.055659
N    -2.530609    -0.283516    -0.024209
 Core  RigidRotor
   SymmetryFactor   1
 End
 Rotor Hindered
 Group 7 9
 Axis 4 1
 Potential[kJ/mol] 72
 0.0
 0.518435320026356
 2.06352484000831
 4.6121504000098
 8.13536515997271
 12.5931525200315
 17.9392241599771
 24.1142751200016
 31.047992559968
 38.6559526600081
 46.8382662799627
 55.476098339966
 64.4288598199921
 73.5282485599896
 82.5759056200297
 91.3229977399794
 99.472962940024
 106.689023219991
 112.695374480001
 117.413839399967
 120.96278791999
 123.513834080035
 125.190036139998
 125.934225040021
 81.4466783000114
 70.1744464199805
 59.630450620034
 49.8218567600304
 37.7298880400019
 28.2866662000288
 19.8321175000046
 12.4161629800142
 6.08539879999626
 0.88194210002257
-3.16189068001336
-6.03110716002107
-7.72900075999132
-8.27981336003631
-7.73012162000555
-6.13767673998495
-3.57309264001628
-0.111360859972365
 4.17178059999515
 9.20187501998839
 14.9053330399966
```

```
 21.2101029400344
 28.0424302599897
 35.3301322399773
 42.9965533399866
 50.9639909999805
 59.1537785800085
 67.4818991599636
 75.8580973799894
 84.186578059979
 92.3473623800135
 100.171810959972
 107.417443899971
 113.735865100034
 118.668425980007
 90.0420476800207
 77.0374287800337
 64.8521146000178
 53.615015999975
 43.3963670400033
 34.2374523400224
 26.1589907800101
 19.1720882600123
 13.2780133200185
 8.47349255998893
 4.75104942002531
 2.10397225998804
 0.523650660028352
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm]      1132.7066
   WellDepth[kJ/mol]     152.80
   WellDepth[kJ/mol]          131.60
   End
   Frequencies[1/cm] 20
176.8495 188.6152 337.7839
431.0837 454.5263 539.0130
552.3565 561.9078 928.1928
1004.5821 1027.6907 1163.2941
1277.9197 1339.1607 1399.4421
1675.3413 2377.5330 3193.1680
3237.5317 3797.8634
   ZeroEnergy[kJ/mol]        -73.10
   ElectronicLevels[1/cm]                     1
      0        2
End
  !*********************************
 Barrier TS5 INT3 P7
 RRHO
  Geometry[angstrom]            9
C    -0.911418    -0.314912    -0.087016
O    -2.187371     0.126116    -0.081448
H    -0.811696    -1.154395     1.549218
C     0.104414     0.552000     0.111747
H    -0.085893     1.574247     0.408131
H    -2.789749    -0.616243    -0.187521
C     1.452092     0.102200     0.004034
N     2.550544    -0.258025    -0.080419
```

```
H    -0.725060    -1.309320    -0.478730
 Core  RigidRotor
   SymmetryFactor   1
 End
 Rotor Hindered
 Group 6 8
 Axis 1 4
 Potential[kJ/mol] 24
 0.0
 4.88679733997964
 19.8201027365685
 44.4155281349784
 76.3147442537587
 91.9794744907802
 91.2265299511137
 69.5404394183666
 43.4284832272013
 20.3078324451242
 2.59075316491224
 -7.86425219257063
 -9.7514228684782
 -2.54609923753298
 13.5250010601904
 37.4939882534694
 67.672350897104
 101.810903165664
 88.117441388147
 76.0142883291344
 57.1061701399517
 35.8955218331025
 17.2453034784595
 4.56195809335238
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 1172.0875
   WellDepth[kJ/mol]    159.70
   WellDepth[kJ/mol]    17.00
   End
   Frequencies[1/cm] 20
 174.2402 176.1744 357.3691
 430.5634 482.3635 496.3392
 533.9950 574.1246 832.2724
 1026.5000 1063.9784 1183.7277
 1222.6019 1345.4755 1362.1333
 1674.7178 2432.7337 3185.7154
 3229.2160 3853.7192
   ZeroEnergy[kJ/mol]        -71.1
   ElectronicLevels[1/cm]                    1
      0        2
End
  !***********************************
 Barrier TS8 INT1 P3
 RRHO
  Geometry[angstrom]            9
C     0.973209    -0.456428    -0.014424
O     2.161746    -0.170047    -0.093295
H     0.648941    -1.485026     0.189502
```

```
C    -0.072654     0.631607    -0.071866
H     0.065333     1.226198    -0.977742
H     0.124238     1.302403     0.776609
H     2.684898     0.765786     0.910022
C    -1.439801     0.121175    -0.002176
N    -2.511700    -0.318159     0.054110
  Core MultiRotor
   SymmetryFactor  1.0
   InterpolationEnergyMax[kJ/mol]  1000
   PotentialEnergySurface[kJ/mol] ./TS8.dat
   InternalRotation
Group    3 7
Axis     1 2
Symmetry            1
     MassExpansionSize 5
     GridSize         100
   End
   InternalRotation
Group   2 8
Axis    1 4
Symmetry            1
     MassExpansionSize 5
     GridSize         100
   End
   End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm]      2023.5248
   WellDepth[kJ/mol]    157.80
   WellDepth[kJ/mol]    41.50
   End
   Frequencies[1/cm] 18
214.2732
350.1666 451.1130 530.6838
658.9097 735.1715 973.2821
1027.8267 1059.2225 1224.4017
1302.6205 1400.1727 1440.4622
1746.6984 2290.6437 3020.9551
3047.5858 3105.0041
   ZeroEnergy[kJ/mol]        -68.10
   ElectronicLevels[1/cm]                      1
      0        2
End
  !*********************************
 Barrier TS10 INT2 INT4
 RRHO
  Geometry[angstrom]            9
C     0.302171    -0.068947     0.490469
O     0.997951    -1.130198    -0.185764
H     0.385532    -0.151275     1.574392
C     1.221740     0.927431    -0.157514
H     0.828727     1.513614    -0.979728
H     1.998643     1.360990     0.460350
H     1.704876    -0.199318    -0.678716
C    -1.111398     0.022089     0.103609
N    -2.229604     0.112745    -0.193324
 Core  RigidRotor
   SymmetryFactor   1
```

```
 End
 Rotor Hindered
 Group 5 6 9
 Axis 1 4
 Potential[kJ/mol] 18
 0.0
 1.56583272520122
 -3.05198596261307
 -4.10440274574545
 3.32886687977174
 15.3285021308439
 17.6038989771894
 7.54679094859423
 -6.44584221874153
 27.2715115269646
 -6.42704752899065
 6.89025819012119
 15.4059708955886
 12.1507874326697
 1.13522766911968
 -7.4575030457187
 -8.35931501190985
 0.753203914369287
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 2114.0032
   WellDepth[kJ/mol]    134.10
   WellDepth[kJ/mol]    209.40
   End
   Frequencies[1/cm] 20
 196.9441 221.9988 381.7461
 528.6942 557.9973 722.2595
 838.4083 962.9805 1010.9513
 1073.0214 1109.6784 1154.9159
 1258.1904 1382.2607 1437.4478
 1997.5196 2278.2297 3108.6690
 3144.5096 3265.0793
   ZeroEnergy[kJ/mol]        -58.50
   ElectronicLevels[1/cm]                      1
      0        2
End
  !***********************************
 Barrier TS12 INT2 INT5
 RRHO
  Geometry[angstrom]            9
C     0.334038    -0.054029     0.133156
O     0.929903    -1.280255    -0.049322
H     0.732929     0.651726     1.118530
C     1.132907     1.179164    -0.041148
H     0.638686     2.112256    -0.261441
H     2.206066     1.076333    -0.087525
H     1.472745    -1.238061    -0.848368
C    -1.091167     0.006170     0.023773
N    -2.249515     0.075763    -0.029666
  Core MultiRotor
   SymmetryFactor  1.0
   InterpolationEnergyMax[kJ/mol]  1000
```

```
   PotentialEnergySurface[kJ/mol] ./TS12.dat
   InternalRotation
Group 7 9
Axis 1 2
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   InternalRotation
Group 8 5
Axis 4 1
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 1972.0316
   WellDepth[kJ/mol]    145.00
   WellDepth[kJ/mol]    122.20
   End
   Frequencies[1/cm] 20
 189.8434 242.4808 291.1496
 391.0150 422.7216 559.6722
 595.3947 669.3678 763.0413
 961.0849 1176.9525 1286.1121
 1308.6600 1390.4744 1433.0032
 2230.9042 2360.3820 3188.9666
 3320.1960 3747.1329
   ZeroEnergy[kJ/mol]        -47.60
   ElectronicLevels[1/cm]                        1
      0        2
End
  !***********************************
 Barrier TS13 INT4 P4
 RRHO
  Geometry[angstrom]            9
C     0.404534     0.110560     0.080546
O     0.933802     1.210862     0.154848
C     1.145341    -1.181204    -0.032381
H     2.198169    -1.021530     0.189752
H     0.716415    -1.928851     0.637712
H     1.425798     1.899735    -1.094031
C    -1.063633     0.018064     0.003480
N    -2.214645    -0.085852    -0.057717
H     1.036995    -1.560560    -1.054883
 Core  RigidRotor
   SymmetryFactor   1
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 1939.2933
   WellDepth[kJ/mol]    38.10
   WellDepth[kJ/mol]    191.80
   End
   Frequencies[1/cm] 20
 102.2311 145.6162 145.6162
 254.4949 434.1059 496.3907
```

```
 602.5216 677.1373 742.8056
 1006.1160 1052.1702 1227.6240
 1405.3450 1468.2553 1480.0857
 1745.1541 2452.8439 3039.2963
 3114.5912 3174.8351
   ZeroEnergy[kJ/mol]        -76.10
   ElectronicLevels[1/cm]                      1
      0        2
End
  !**********************************
 Barrier TS14 INT5 P4
 RRHO
  Geometry[angstrom]            9
C    -0.425636     0.206064     0.067193
O    -0.871318     1.326935    -0.092143
C    -1.245792    -1.060924    -0.058808
H    -1.215910    -1.353930    -1.112469
H    -0.828902    -1.873967     0.534548
C     1.052289    -0.019362     0.007310
N     2.193482    -0.223158    -0.065974
H    -2.275369    -0.855081     0.226532
H    -0.355032     0.187132     1.736063
 Core  RigidRotor
   SymmetryFactor   1
 End
 Rotor Hindered
 Group 2 8
 Axis 1 3
 Potential[kJ/mol] 24
 0.0
 1.27194123824603
 4.44118267947204
 7.6804566023956
 9.03623703701311
 7.85677705572703
 4.95433425888599
 1.83396735938909
 0.075316847379448
 0.803481914799235
 3.95391396483585
 7.63256836704718
 9.02745085035093
 7.44104272821847
 4.33249759200006
 1.40067037196798
 0.016259223342914
 0.990109624703408
 4.092344184944
 7.59719837380859
 9.03438387305732
 7.51370597292085
 4.27549580132935
 1.23702725090021
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 1383.6046
   WellDepth[kJ/mol]    92.40
```

```
   WellDepth[kJ/mol]    33.30
   End
   Frequencies[1/cm] 20
 174.0690 187.1979 265.0230
 421.5212 506.0490 543.2105
 610.1661 627.6835 728.8824
 1002.8822 1055.3619 1186.0447
 1403.1669 1479.0501 1486.8348
 1742.5459 2258.4587 3054.8681
 3137.3841 3178.0182
   ZeroEnergy[kJ/mol]        -77.40
   ElectronicLevels[1/cm]                    1
      0        2
End
  !**********************************
 Barrier TS15 INT5 P5
 RRHO
  Geometry[angstrom]            9
C    -0.310687     0.527182     0.408540
O    -0.868530     1.354743    -0.294369
C    -1.281700    -1.294700    -0.095820
H    -1.035936    -1.322914    -1.148311
H    -0.764334    -1.986617     0.557108
C     1.047279     0.024054     0.078946
N     2.112807    -0.374459    -0.155865
H    -2.289028    -1.004616     0.168934
H    -0.591439     0.351855     1.457777
 Core  RigidRotor
   SymmetryFactor   1
 End
 Rotor Hindered
 Group 2 8
 Axis 1 3
 Potential[kJ/mol] 24
 0.0
 0.837700473432463
 2.88165317956669
 4.96293405290399
 5.84277713951649
 4.98632004242865
 2.91552494264156
 0.861326148269313
 0.000788887638976
 0.800416935455104
 2.80723810557623
 4.89198640913928
 5.83928004399593
 5.0764440873165
 3.04796066684208
 0.946550426562126
 0.002563031614521
 0.775205872091355
 2.82282736510102
 4.93997387891793
 5.84173202745631
 4.9779872363624
 2.89136345423071
```

```
 0.8405192043342
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 490.6525
   WellDepth[kJ/mol]    68.20
   WellDepth[kJ/mol]    9.10
   End
   Frequencies[1/cm] 20
 143.6317 150.1111 236.1380
 291.3741 433.0453 593.7990
 614.6141 630.9230 904.2265
 932.4602 1044.3170 1387.4141
 1432.6508 1446.8454 1627.8504
 2263.1225 3000.2002 3108.4727
 3279.5266 3290.5715
   ZeroEnergy[kJ/mol]        -101.60
   ElectronicLevels[1/cm]                      1
      0        2
End
  !***********************************
 Barrier TS16 INT2 P2
 RRHO
  Geometry[angstrom]            9
C     0.436290     0.033779     0.059402
O     0.996474    -1.197203    -0.142723
H     0.329343    -0.013623     1.856427
C     1.172628     1.151842    -0.077762
H     0.693242     2.117949    -0.053825
H     2.248480     1.081821    -0.148338
H     0.412434    -1.880038     0.205614
C    -1.015941     0.089477    -0.006934
N    -2.172698     0.084454    -0.074650
  Core MultiRotor
   SymmetryFactor  1.0
   InterpolationEnergyMax[kJ/mol]  1000
   PotentialEnergySurface[kJ/mol] ./TS16.dat
   InternalRotation
Group 7
Axis 1 2
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   InternalRotation
Group 5 6 9
Axis 1 4
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 1279.0235
   WellDepth[kJ/mol]    146.00
   WellDepth[kJ/mol]    33.20
   End
   Frequencies[1/cm] 20
```

```
  189.2045 286.3709 298.5808
  421.2752 514.1961 529.0157
  616.8174 662.7227 696.8953
  807.6498 906.0247 985.7958
  1247.0125  1322.9145 1436.8579
  1645.0141  2383.4583 3195.2091
  3306.7626 3826.3145
    ZeroEnergy[kJ/mol]        -46.60
    ElectronicLevels[1/cm]                      1
       0        2
 End
End
```

5.2 *Anti*-VyA + CN

```
!************************************************
!               GLOBAL SECTION
!************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]                      30 40 50 60 70 80 90 100 110 120
                                        130 140 150 160 170 180
                                        190 200 210 220 230 240
                                        250 260 270 280 290 300
                                        310 320 330 340 350 360
                                        370 380 390 400 410 420
                                        430 440 450 460 470 480
                                        490 500 510 520 530 540
                                        550 560 570 580 590 600
PressureList[atm]                       1.e-8 1
EnergyStepOverTemperature               .2
ExcessEnergyOverTemperature             30
ModelEnergyLimit[kcal/mol]              400
CalculationMethod                       low-eigenvalue
WellCutoff                              20
ChemicalEigenvalueMax                   0.2
ReductionMethod                         projection
AtomDistanceMin[bohr]                  1.3
RateOutput                              rate.out


!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!************************************************
!               MODEL SECTION
!************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

Model
  EnergyRelaxation
    Exponential
       Factor[1/cm]                     260
       Power                            0.85
       ExponentCutoff                   15
End

CollisionFrequency
```

```
    LennardJones
       Epsilons[K]                      127.697  1280.940
       Sigmas[angstrom]                 3.462    4.495
       Masses[amu]                      39.948 70.07098
   End

!************************************************
!
!************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!************************************************
!  REACTANT syn-Vy + CN
!************************************************
 Bimolecular REACS
 Fragment C2H4O
 RRHO
 Geometry[angstrom]               7
 C     0.035965     0.414901     0.000010
 O    -1.132689    -0.296697     0.000001
 H    -0.067014     1.495467     0.000038
 C     1.225337    -0.181204    -0.000014
 H     1.314586    -1.259393    -0.000042
 H     2.120535     0.422594    -0.000006
 H    -1.874405     0.312722     0.000028
 Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]       15
  274.4399 479.1481 718.0128
  855.2196 961.1790 976.6347
  1145.8603 1295.2582 1351.8397
  1446.9336 1727.9531 3169.9747
  3186.3356 3281.3570 3876.6283
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                     1
   0            1
 !***********************************
 End
!*********
 Fragment CN
 RRHO
 Geometry[angstrom]               2
 C    -1.875383     0.453789     0.017829
 N    -0.716421     0.453789     0.017829
Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]   1
  2411.1619
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                     1
   0            2
 !***********************************
 End
!*********
GroundEnergy[kJ/mol] 0.0
End
```

```
!************************************************
!  PRODUCT P1
!************************************************
 Bimolecular P1
 Fragment C3H3NO
 RRHO
 Geometry[angstrom]                8
 C     -2.382269      0.945131     -0.000362
 H     -2.955911      0.024193     -0.000477
 C     -1.042183      0.938093     -0.000079
 H     -0.479726      1.862579      0.000035
 O     -3.073123      2.105766     -0.000511
 H     -4.016875      1.922791     -0.000715
 C     -0.329433     -0.294769      0.000078
 N      0.266749     -1.294247      0.000210
 Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    18
 177.5084 194.3963 364.1156
 441.7379 516.5180 559.1184
 828.9453 964.4885 1025.9549
 1180.2978 1229.4947 1356.0995
 1363.8277 1729.7660 2261.0347
 3189.9610 3217.6987 3861.8155
  ZeroEnergy[kJ/mol]              0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        1.0000000000000000
    !***********************************
 End
!*********
 Fragment HYDROGEN
  Atom
  Name H
  ElectronicLevels[1/cm]       1
   0       2
   !***********************************
 End
!*********
GroundEnergy[kJ/mol] -98.60
End
!************************************************
!  PRODUCT P2
!************************************************
 Bimolecular P2
 Fragment C3H3NO
 RRHO
 Geometry[angstrom]                8
 C      0.443981      0.039262     -0.000001
 C      1.198529      1.140439      0.000000
 H      2.276862      1.062360      0.000002
 O      0.990152     -1.212171     -0.000000
 H      0.291376     -1.874294      0.000005
 C     -0.994930      0.104485     -0.000001
 N     -2.157744      0.098859      0.000001
 H      0.729281      2.112173      0.000000
  Core  RigidRotor
```

```
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    18
  193.3575 232.2772 291.3889
  422.2905 608.0666 637.7575
  739.3691 797.2002 886.2303
  985.2469 1240.7954 1342.9461
  1440.1943 1714.9378 2258.4905
  3190.6084 3296.5683 3843.1869
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        1.0000000000000000
    !***********************************
 End
!*********
 Fragment HYDROGEN
  Atom
  Name H
  ElectronicLevels[1/cm]       1
   0       2
   !***********************************
 End
!*********
GroundEnergy[kJ/mol] -85.10
End
!************************************************
!  PRODUCT P3
!************************************************
 Bimolecular P3
 Fragment C3H3NO
 RRHO
 Geometry[angstrom]               8
 C    -1.345923     0.104809    -0.027948
 N    -2.377393    -0.417343    -0.125136
 C    -0.023598     0.714489     0.099916
 H     0.191721     1.363573    -0.749015
 H    -0.003508     1.324207     1.009576
 C     1.076489    -0.337387     0.222890
 O     2.175451    -0.176213    -0.242639
 H     0.808118    -1.248133     0.787358
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    18
  61.1798 181.1152 351.3555
  469.1521 521.0854 737.8674
  964.6614 1046.0583 1050.0161
  1227.9169 1297.3395 1419.0734
  1451.8066 1794.2927 2284.8892
  2973.3366 3061.7878 3137.0962
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        1.0000000000000000
    !***********************************
 End
!*********
 Fragment HYDROGEN
```

```
  Atom
  Name H
  ElectronicLevels[1/cm]       1
   0       2
   !***********************************
 End
!*********
GroundEnergy[kJ/mol] -114.90
End
!************************************************
!  PRODUCT P4
!************************************************
 Bimolecular P4
 Fragment C3H3NO
 RRHO
 Geometry[angstrom]               8
 C     0.435388     0.206437    -0.000013
 O     0.875395     1.331535    -0.000061
 C    -1.033749    -0.009358     0.000014
 N    -2.179015    -0.205280     0.000032
 C     1.253779    -1.050580     0.000026
 H     1.002871    -1.648213     0.879919
 H     1.002857    -1.648277    -0.879819
 H     2.311705    -0.797822     0.000008
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    18
  136.5165 177.0018 250.3718
  433.1108 589.6386 595.9424
  724.1801 993.0990 1050.8204
  1209.4700 1405.3542 1472.7222
  1480.6838 1770.4367 2246.8223
  3053.6406 3124.0572 3176.6486
  ZeroEnergy[kJ/mol]              0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        1.0000000000000000
    !***********************************
 End
!*********
 Fragment HYDROGEN
  Atom
  Name H
  ElectronicLevels[1/cm]       1
   0       2
   !***********************************
 End
!*********
GroundEnergy[kJ/mol] -119.50
End
!************************************************
!  PRODUCT P5
!************************************************
 Bimolecular P5
 Fragment C2HNO
 RRHO
 Geometry[angstrom]               5
```

```
 C    -0.692079     0.426205    -0.000021
 O    -1.562173    -0.407499     0.000045
 C     0.737630     0.069129    -0.000014
 N     1.873815    -0.174115    -0.000009
 H    -0.892626     1.506792    -0.000090
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    9
  224.6826 297.9226 616.1239
  927.4680 998.9194 1413.0009
  1751.8461 2250.0589 3033.9889
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                     1
   0.0000000000000000        1.0000000000000000
    !***********************************
 End
!*********
  Fragment CH3
  RRHO
  Geometry[angstrom]               4
 C    -0.204697     0.140730    -0.218631
 H     0.303637    -0.757915     0.092664
 H     0.303657     0.859632    -0.841227
 H    -1.221388     0.320469     0.092664
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    6
  488.3360 1430.3272 1430.3273
  3136.9147 3319.3943 3319.3943
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]       1
   0       2
   !***********************************
 End
!*********
GroundEnergy[kJ/mol] -116.00
End
!************************************************
!  PRODUCT P6
!************************************************
 Bimolecular P6
 Fragment C3H3N
 RRHO
 Geometry[angstrom]               7
 C    -0.608242     0.671357     0.000006
 H    -1.181236    -0.247803     0.000007
 C     0.727830     0.662097     0.000002
 H     1.269248    -0.274564     0.000000
 H     1.298781     1.581579     0.000001
 C    -1.365754     1.888472     0.000009
 N    -1.997712     2.864467     0.000012
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    15
```

```
  230.6762 340.8485 566.7814
  702.0030 880.3037 987.8886
  1010.4583 1111.1755 1322.6420
  1453.7345 1675.5742 2263.3312
  3172.0516 3204.5565 3270.4973
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        1.0000000000000000
    !***********************************
 End
!*********
  Fragment HO
  RRHO
  Geometry[angstrom]               2
 O    -1.121951     0.449697    -0.040988
 H    -1.446314     1.365670    -0.040988
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    1
  3757.1215
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]       1
   0       2
   !***********************************
 End
!*********
GroundEnergy[kJ/mol] -101.50
End
!************************************************
!  PRODUCT P7
!************************************************
 Bimolecular P7
 Fragment C3H3NO
 RRHO
 Geometry[angstrom]               8
 C    -2.378164     1.002522     0.000021
 C    -1.037611     1.032446     0.001148
 O    -3.122332     2.127217     0.000016
 H    -4.056895     1.902113    -0.000884
 H    -0.492664     0.099905     0.001093
 C    -0.293089     2.247818     0.002424
 N     0.338404     3.224906     0.003476
 H    -2.907880     0.056270    -0.000931
 Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]    18
  149.3755 270.1390 371.8154
  405.5380 590.2572 728.6013
  744.5695 949.8776 952.8482
  1118.2506 1256.9964 1305.2108
  1437.4753 1726.3904 2260.3805
  3191.4026 3239.6076 3862.2591
  ZeroEnergy[kJ/mol]             0.
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        1.0000000000000000
```

```
    !***********************************
 End
!*********
 Fragment HYDROGEN
  Atom
  Name H
  ElectronicLevels[1/cm]       1
   0       2
   !***********************************
 End
!*********
GroundEnergy[kJ/mol] -109.40
End
!************************************************
!  INT1
!************************************************
 Well INT1
 Species
 RRHO     ! well
 Geometry[angstrom]               9
 C    -1.150932     0.386547    -0.375960
 O    -1.673440    -0.666779     0.316802
 H    -1.273802     0.390953    -1.453333
 C     0.096160     0.936729     0.235924
 H    -0.041662     1.053629     1.313575
 H     0.313950     1.920135    -0.184541
 H    -2.377469    -1.073997    -0.196910
 C     1.265314     0.068067     0.007300
 N     2.169367    -0.628796    -0.203783
 Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]            21
 90.2495 192.4609 355.2716
 370.9197 385.7554 547.5608
 686.0015 892.0347 917.4241
 1031.7060 1199.8734 1230.3189
 1311.9987 1329.0932 1458.1137
 1464.5611 2271.7296 3072.9575
 3124.8619 3178.8569 3852.2232
  ZeroEnergy[kJ/mol]     -230.30
  ElectronicLevels[1/cm]                     1
   0.0000000000000000        2.0000000000000000
 End
 End
!************************************************
!  INT1b
!************************************************
 Well INT1b
 Species
 RRHO     ! well
 Geometry[angstrom]               9
 C     0.607662     0.081245     0.484541
 O     1.606201    -0.525769    -0.260327
 H     0.752419     0.120428     1.561019
 C    -0.106259     1.228763    -0.169707
 H     0.170229     1.443178    -1.195284
```

```
 H    -0.407234     2.069767     0.442932
 H     1.605880    -1.469028    -0.065629
 C    -0.847937    -0.061981     0.028439
 N    -1.815698    -0.780466    -0.084464
 Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]            21
 193.0045 303.4894 341.8641
 407.9997 480.9786 632.8671
 744.7724 853.2031 947.4853
 1046.2651 1060.5644 1126.4644
 1202.6223 1291.0868 1403.4067
 1450.6352 1912.9179 3140.8465
 3143.1149 3245.5677 3827.3069
  ZeroEnergy[kJ/mol]      -115.10
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        2.0000000000000000
 End
 End
!************************************************
!  INT2
!************************************************
 Well INT2
 Species
 RRHO     ! well
 Geometry[angstrom]               9
 C     0.424723    -0.018446     0.383703
 O     1.006460    -1.208950    -0.140369
 H     0.560788    -0.108137     1.466272
 C     1.086852     1.217589    -0.126004
 H     2.154941     1.311218     0.005584
 H     0.522218     2.012839    -0.587756
 H     0.992787    -1.145271    -1.102593
 C    -1.033056     0.018850     0.124049
 N    -2.170629     0.053585    -0.102315
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]            21
  65.8557 190.8567 232.0591
  334.9546 393.3755 509.3741
  574.5730 613.0193 807.2125
  976.1030 1089.5257 1125.7179
  1237.7492 1346.9905 1413.0694
  1469.2960 2274.6364 3057.1023
  3184.8072 3308.6257 3809.8375
  ZeroEnergy[kJ/mol]      -197.90
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        2.0000000000000000
 End
 End
!************************************************
!  INT3
!************************************************
 Well INT3
 Species
```

```
 RRHO     ! well
 Geometry[angstrom]                9
 C     0.988855    -0.451602     0.291772
 O     2.181772     0.091644    -0.250676
 H     0.700065    -1.384477    -0.203082
 C    -0.141240     0.528383     0.246121
 H     0.057252     1.572710     0.446049
 H     2.046477     0.238001    -1.192277
 C    -1.461617     0.120365     0.020576
 N    -2.547823    -0.241163    -0.175942
 H     1.225660    -0.692625     1.332968
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]             21
  47.0339 185.5126 325.0330
  394.7722 428.4037544.6996
  577.9890 887.5487 1041.8618
  1071.4663 1120.2467 1195.5659
  1320.2677 1398.8290 1428.7017
  1498.8184 2316.6123 3036.8405
  3078.0715 3225.4018 3834.6120
  ZeroEnergy[kJ/mol]       -234.70
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        2.0000000000000000
 End
 End
!************************************************
!  INT4
!************************************************
 Well INT4
 Species
 RRHO     ! well
 Geometry[angstrom]                9
 C     0.338179     0.053219     0.000062
 O     0.862528     1.306811     0.000292
 C     1.325205    -1.052983     0.000045
 H     1.968304    -0.991214     0.883150
 H     0.816834    -2.015413    -0.000143
 H     0.152117     1.959414     0.000287
 C    -1.050149    -0.116959    -0.000144
 N    -2.208459    -0.235861    -0.000314
 H     1.968528    -0.990987    -0.882881
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]             21
  90.6477 190.0395 238.3457
  385.8546 404.4841 461.3178
  621.5631 749.7738 1015.0283
  1023.8833 1172.6828 1366.3166
  1411.4686 1441.0116 1478.6647
  1511.7408 2329.9872 3034.6289
  3090.0035 3159.0180 3814.6683
  ZeroEnergy[kJ/mol]       -273.20
  ElectronicLevels[1/cm]                      1
   0.0000000000000000        2.0000000000000000
```

```
 End
 End
!************************************************
!  INT5
!************************************************
 Well INT5
 Species
 RRHO     ! well
 Geometry[angstrom]               9
 C     0.409848    -0.041316     0.380390
 O     1.041703    -1.144416    -0.140658
 C     1.125194     1.214977    -0.154543
 H     1.065265     1.238867    -1.241852
 H     0.635570     2.101157     0.248889
 C    -1.038927     0.003264     0.057753
 N    -2.171740     0.059832    -0.186926
 H     2.168228     1.191981     0.156014
 H     0.521602    -0.063452     1.472807
  Core  RigidRotor
  SymmetryFactor    1.0000000000000000
  End
     Frequencies[1/cm]            21
  185.9006 214.4629 245.7042
  293.8295 505.1179 579.8116
  800.6449 894.3748 985.6645
  1041.5556 1122.4717 1232.4704
  1350.7839 1406.0258 1493.4699
  1510.1447 2273.0772 3017.1289
  3071.1608 3161.0452 3171.1542
  ZeroEnergy[kJ/mol]      -175.10
  ElectronicLevels[1/cm]                     1
   0.0000000000000000        2.0000000000000000
 End
 End
!************************************************
!  BARRIERLESS ENTRANCE CHANNEL - PHASE SPACE THEORY
!************************************************
 Barrier B0 REACS INT1
   RRHO
     Stoichiometry  C3H4N1O1
     Core PhaseSpaceTheory
       FragmentGeometry[angstrom]               7
 C     0.035965     0.414901     0.000010
 O    -1.132689    -0.296697     0.000001
 H    -0.067014     1.495467     0.000038
 C     1.225337    -0.181204    -0.000014
 H     1.314586    -1.259393    -0.000042
 H     2.120535     0.422594    -0.000006
 H    -1.874405     0.312722     0.000028
       FragmentGeometry[angstrom]               2
 C    -1.875383     0.453789     0.017829
 N    -0.716421     0.453789     0.017829
SymmetryFactor     1.0000000000000000
           PotentialPrefactor[au]     63.49
           PotentialPowerExponent  6
      End
     Frequencies[1/cm]            16
```

```
 274.4399 479.1481 718.0128
 855.2196 961.1790 976.6347
 1145.8603 1295.2582 1351.8397
 1446.9336 1727.9531 3169.9747
 3186.3356 3281.3570 3876.6283
 2411.1619
 ZeroEnergy[kJ/mol]            0.
 ElectronicLevels[1/cm]                   1
  0.0000000000000000        2.0000000000000000
   End
!***********************************
 Barrier TS1 INT1 INT1b
 RRHO
  Geometry[angstrom]             9
C     0.667077     0.096591     0.485498
O     1.634643    -0.636635    -0.148131
H     0.807100     0.126835     1.556499
C    -0.094898     1.197815    -0.185872
H     0.167373     1.426518    -1.215603
H    -0.355272     2.063858     0.415481
H     1.427359    -0.716241    -1.085950
C    -0.934516    -0.001828    -0.000229
N    -1.827872    -0.791445    -0.050937
 Core  RigidRotor
   SymmetryFactor   1
 End
 Rotor Hindered
 Group 7
 Axis 1 2
 Potential[kJ/mol] 24
 0.0
 0.384531131041655
 1.47030644085475
 2.89502436536483
 4.31435212655795
 5.6060688479987
 6.79707940421117
 7.8849866795811
 8.74069374275182
 9.06711207726815
 8.43506397539111
 6.49114222014795
 3.19850930340067
 -0.960534345751633
 -5.07495242028298
 -8.14490401874958
 -9.42151925209061
 -8.6796217644428
 -6.31733649378974
 -3.27931161061933
 -0.698192063120729
 0.661604741482321
 0.780898464158717
 0.297642969226459
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 577.5630
```

```
    WellDepth[kJ/mol]    123.20
    WellDepth[kJ/mol]    8.0
    End
    Frequencies[1/cm] 20
  138.0329 249.1384 337.9022
  415.4476 478.4118 783.9889
  849.4804 941.7737 1007.2288
  1077.2953 1117.7864 1207.2879
  1324.7120 1423.5397 1453.1612
  2030.3371 3108.0357 3199.1384
  3229.6599 3820.9414
    ZeroEnergy[kJ/mol]        -107.10
    ElectronicLevels[1/cm]                    1
       0        2
End
  !***********************************
  Barrier TS1b INT1b INT2
  RRHO
   Geometry[angstrom]            9
C      0.567096     0.035035     0.461466
O      1.512286    -0.722091    -0.229405
H      0.712619     0.082565     1.540513
C      0.009785     1.273776    -0.165612
H      0.165385     1.425643    -1.224305
H     -0.316229     2.095358     0.455608
H      2.297633    -0.175153    -0.345094
C     -0.830667    -0.191724     0.084663
N     -1.919283    -0.622029    -0.124941
  Core         RigidRotor
    SymmetryFactor   1
  End
  Rotor Hindered
  Group 7
  Axis 1 2
  Potential[kJ/mol] 24
  0.0
  0.489270730274633
  1.89197199562412
  3.70901043041916
  5.04851037719963
  5.00146143429436
  3.18676419744718
  0.033827921400906
  -3.41981157783085
  -6.04393324540262
  -7.09080733819441
  -6.46648009661861
  -4.74323869406182
  -2.8628469386589
  -1.66592431936764
  -1.39529596020829
  -1.59447630297682
  -1.55602531634445
  -0.874531418291028
  0.290695245081544
  1.33462459496117
  1.65246256235773
```

```
 1.16385733293389
 0.37928981933274
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm]   677.9480
   WellDepth[kJ/mol]   15.50
   WellDepth[kJ/mol]   98.30
   End
   Frequencies[1/cm] 20
211.4278 226.3736 351.7120
406.1711 492.1999 745.8929
824.8348 873.6945 894.5697
1080.2098 1167.7307 1205.7098
1306.4266 1393.4610 1449.8594
2042.6957 3107.2677 3170.6329
3294.3832 3813.4662
   ZeroEnergy[kJ/mol]       -107.10
   ElectronicLevels[1/cm]                      1
      0        2
End
  !**********************************
 Barrier TS3 INT1 INT3
 RRHO
  Geometry[angstrom]            9
C     1.250669     0.421444    -0.080454
O     1.448643    -0.922534    -0.134443
H     2.114504     1.008116     0.195654
C    -0.102803     0.996542     0.152658
H     0.500170     1.057870    -0.988633
H    -0.181906     1.956790     0.641123
H     0.610965    -1.384199     0.013819
C    -1.210093     0.115617     0.129903
N    -2.059686    -0.679345     0.077561
  Core MultiRotor
   SymmetryFactor  1.0
   InterpolationEnergyMax[kJ/mol]  1000
   PotentialEnergySurface[kJ/mol] ./TS3.dat
   InternalRotation
Group  7
Axis  1 2
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   InternalRotation
Group  7 9
Axis  4 1
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 1924.2687
   WellDepth[kJ/mol]    164.10
   WellDepth[kJ/mol]    168.50
   End
```

```
   Frequencies[1/cm] 20
 130.8542 206.6971 331.0802
 412.6942 432.8810 657.4672
 683.1535 813.3618 895.1560
 1076.6411 1193.8244 1273.1801
 1327.2376 1359.2747 1433.7286
 2145.0885 2327.6981 3224.0019
 3234.3662 3749.8659
   ZeroEnergy[kJ/mol]        -66.20
   ElectronicLevels[1/cm]                      1
      0        2
End
  !**********************************
 Barrier TS3b INT2 P6
 RRHO
  Geometry[angstrom]            9
C     0.255727     0.377936     0.511840
O     1.217745    -1.312316    -0.036073
H     0.515450     0.158045     1.537357
C     1.023432     1.184436    -0.249777
H     0.702847     1.496782    -1.234800
H     1.999153     1.490612     0.098749
H     1.018149    -1.323017    -0.985933
C    -1.099169     0.063911     0.121422
N    -2.190669    -0.166943    -0.188721
  Core MultiRotor
   SymmetryFactor  1.0
   InterpolationEnergyMax[kJ/mol]  1000
   PotentialEnergySurface[kJ/mol] ./TS3b.dat
   InternalRotation
Group  7
Axis 1 2
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   InternalRotation
Group  6 8
Axis  4 1
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 552.4366
   WellDepth[kJ/mol]    105.50
   WellDepth[kJ/mol]    9.10
   End
   Frequencies[1/cm] 20
 144.9891 171.3810 223.1567
 281.2298 429.4659 567.6507
 670.0482 796.9721 875.3571
 974.7342 1047.7554 1114.9621
 1310.1136 1454.4357 1640.7606
 2416.6629 3180.9562 3233.0109
 3288.9018 3757.0446
```

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   ZeroEnergy[kJ/mol]        -92.40
   ElectronicLevels[1/cm]                      1
      0        2
End
  !***********************************
 Barrier TS4 INT1 P1
 RRHO
  Geometry[angstrom]            9
 C     0.932324    -0.356049     0.095185
 O     2.211832     0.008191    -0.097272
 H     0.743844    -1.349749     0.485472
 C    -0.068127     0.520948    -0.119763
 H     0.123225     1.456674    -0.627959
 H    -0.169327     1.569052     1.401728
 H     2.800709    -0.710917     0.150147
 C    -1.424189     0.056413    -0.047216
 N    -2.520454    -0.317557     0.002945
 Core  RigidRotor
 SymmetryFactor   1
 End
 Rotor Hindered
 Group 7 9
 Axis 1 2
 Potential[kJ/mol] 71
 0.0
 0.59625097997582
 2.397917339988
 5.41891505998251
 9.66757115999712
 15.1459804599881
 21.8523572800109
 29.7758250399738
 38.9004304000025
 49.1981099999919
 60.6221114199855
 73.0912608399592
 86.4504989399507
 100.329043880004
 113.033713519951
 121.384234139958
 126.285356079995
 128.336584739998
 107.174738319975
 98.648555459954
 89.7464586199817
 80.7054481999558
 71.7082789799917
 62.9006068600177
 54.4030567599918
 46.3184667400128
 38.7369847799789
 31.738990399964
 25.3946778799843
 19.7665478400154
 14.9096989599514
 10.8744797199677
 7.70339933996524
```

```
 5.43433305994654
 4.09732777998215
 3.72064030000843
 4.327261639946
 5.93561566001313
 8.56333763998691
 12.223210999997
 16.9253913400155
 22.6801964999538
 29.4931558999508
 37.3645578800165
 46.2943189799546
 56.2772576599969
 67.2977559799733
 79.3375416599702
 92.3635437400037
 106.32725584
 121.146581140016
 136.650856679989
 127.82194749999
 129.389225679984
 114.65340119999
 109.383883700019
 103.114494080018
 95.8345036999845
 87.6758375999543
 78.8868573999935
 69.7464055599653
 60.5167074199471
 51.4286718400115
 42.6805693599874
 34.4435899599944
 26.8618734799873
 20.0573258599888
 14.1253821799978
 9.15338293998502
 5.20469638000236
 2.3354921199541
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm]   1130.2824
   WellDepth[kJ/mol]    153.10
   WellDepth[kJ/mol]    21.40
   End
   Frequencies[1/cm] 20
 176.9677 197.0173 349.6582
 381.0129 442.2342 487.2426
 542.0210 563.8588 917.9680
 995.4219 1019.5905 1182.9001
 1237.7799 1353.5869 1362.6240
 1708.4642 2383.7014 3200.2767
 3218.0276 3855.5901
   ZeroEnergy[kJ/mol]       -77.20
   ElectronicLevels[1/cm]                      1
      0        2
End
  !*********************************
```

```
 Barrier TS5 INT3 P7
 RRHO
  Geometry[angstrom]            9
C    -0.905315    -0.314056    -0.082033
O    -2.182927     0.122117    -0.089299
H    -0.800137    -1.097928     1.581223
C     0.107487     0.562830     0.086076
H    -0.086297     1.593702     0.348374
H    -2.782624    -0.625632    -0.169561
C     1.456715     0.114741    -0.008562
N     2.556411    -0.243981    -0.082571
H    -0.715719    -1.320310    -0.440533
 Core  RigidRotor
   SymmetryFactor   1
 End
 Rotor Hindered
 Group 6 8
 Axis 1 2
 Potential[kJ/mol] 24
 0.0
 4.88679733997964
 19.8201027365685
 44.4155281349784
 76.3147442537587
 91.9794744907802
 91.2265299511137
 69.5404394183666
 43.4284832272013
 20.3078324451242
 2.59075316491224
 -7.86425219257063
 -9.7514228684782
 -2.54609923753298
 13.5250010601904
 37.4939882534694
 67.672350897104
 101.810903165664
 88.117441388147
 76.0142883291344
 57.1061701399517
 35.8955218331025
 17.2453034784595
 4.56195809335238
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm]    1172.0875
   WellDepth[kJ/mol]    157.80
   WellDepth[kJ/mol]    32.50
   End
   Frequencies[1/cm] 20
174.2402 176.1744 357.3691
430.5634 482.3635 496.3392
533.9950 574.1246 832.2724
1026.5000 1063.9784 1183.7277
1222.6019 1345.4755 1362.1333
1674.7178 2432.7337 3185.7154
3229.2160 3853.7192
```

```
   ZeroEnergy[kJ/mol]        -76.90
   ElectronicLevels[1/cm]                      1
      0        2
End
  !**********************************
 Barrier TS8 INT1 P3
 RRHO
  Geometry[angstrom]            9
C     0.973209    -0.456428    -0.014424
O     2.161746    -0.170047    -0.093295
H     0.648941    -1.485026     0.189502
C    -0.072654     0.631607    -0.071866
H     0.065333     1.226198    -0.977742
H     0.124238     1.302403     0.776609
H     2.684898     0.765786     0.910022
C    -1.439801     0.121175    -0.002176
N    -2.511700    -0.318159     0.054110
  Core MultiRotor
   SymmetryFactor  1.0
   InterpolationEnergyMax[kJ/mol]  1000
   PotentialEnergySurface[kJ/mol] ./TS8.dat
   InternalRotation
Group    3 7
Axis     1 2
Symmetry            1
     MassExpansionSize 5
     GridSize         100
   End
   InternalRotation
Group   2 8
Axis    1 4
Symmetry            1
     MassExpansionSize 5
     GridSize         100
   End
   End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm]      2023.5248
   WellDepth[kJ/mol]    156.90
   WellDepth[kJ/mol]    41.50
   End
   Frequencies[1/cm] 20
70.8016 160.4364 214.2732
350.1666 451.1130 530.6838
658.9097 735.1715 973.2821
1027.8267 1059.2225 1224.4017
1302.6205 1400.1727 1440.4622
1746.6984 2290.6437 3020.9551
3047.5858 3105.0041
   ZeroEnergy[kJ/mol]        -73.40
   ElectronicLevels[1/cm]                      1
      0        2
End
  !**********************************
 Barrier TS10 INT2 INT4
 RRHO
  Geometry[angstrom]            9
```

```
C     0.302171    -0.068947     0.490469
O     0.997951    -1.130198    -0.185764
H     0.385532    -0.151275     1.574392
C     1.221740     0.927431    -0.157514
H     0.828727     1.513614    -0.979728
H     1.998643     1.360990     0.460350
H     1.704876    -0.199318    -0.678716
C    -1.111398     0.022089     0.103609
N    -2.229604     0.112745    -0.193324
 Core  RigidRotor
   SymmetryFactor   1
 End
 Rotor Hindered
 Group 5 6 9
 Axis 1 4
 Potential[kJ/mol] 18
 0.0
 1.56583272520122
 -3.05198596261307
 -4.10440274574545
 3.32886687977174
 15.3285021308439
 17.6038989771894
 7.54679094859423
 -6.44584221874153
 27.2715115269646
 -6.42704752899065
 6.89025819012119
 15.4059708955886
 12.1507874326697
 1.13522766911968
 -7.4575030457187
 -8.35931501190985
 0.753203914369287
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 2114.0032
   WellDepth[kJ/mol]    134.10
   WellDepth[kJ/mol]    209.40
   End
   Frequencies[1/cm] 20
 196.9441 221.9988 381.7461
 528.6942 557.9973 722.2595
 838.4083 962.9805 1010.9513
 1073.0214 1109.6784 1154.9159
 1258.1904 1382.2607 1437.4478
 1997.5196 2278.2297 3108.6690
 3144.5096 3265.0793
   ZeroEnergy[kJ/mol]        -63.80
   ElectronicLevels[1/cm]                      1
      0        2
End
  !**********************************
 Barrier TS12 INT2 INT5
 RRHO
  Geometry[angstrom]            9
C     0.334038    -0.054029     0.133156
```

```
O     0.929903    -1.280255    -0.049322
H     0.732929     0.651726     1.118530
C     1.132907     1.179164    -0.041148
H     0.638686     2.112256    -0.261441
H     2.206066     1.076333    -0.087525
H     1.472745    -1.238061    -0.848368
C    -1.091167     0.006170     0.023773
N    -2.249515     0.075763    -0.029666
  Core MultiRotor
   SymmetryFactor  1.0
   InterpolationEnergyMax[kJ/mol]  1000
   PotentialEnergySurface[kJ/mol] ./TS12.dat
   InternalRotation
Group 7 9
Axis 1 2
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   InternalRotation
Group 8 5
Axis 4 1
Symmetry            1
     MassExpansionSize 3
     GridSize         100
   End
   End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 1972.0316
   WellDepth[kJ/mol]    144.30
   WellDepth[kJ/mol]    122.20
   End
   Frequencies[1/cm] 20
 189.8434 242.4808 291.1496
 391.0150 422.7216 559.6722
 595.3947 669.3678 763.0413
 961.0849 1176.9525 1286.1121
 1308.6600 1390.4744 1433.0032
 2230.9042 2360.3820 3188.9666
 3320.1960 3747.1329
   ZeroEnergy[kJ/mol]        -52.90
   ElectronicLevels[1/cm]                      1
      0        2
End
  !***********************************
 Barrier TS13 INT4 P4
 RRHO
  Geometry[angstrom]            9
C     0.404534     0.110560     0.080546
O     0.933802     1.210862     0.154848
C     1.145341    -1.181204    -0.032381
H     2.198169    -1.021530     0.189752
H     0.716415    -1.928851     0.637712
H     1.425798     1.899735    -1.094031
C    -1.063633     0.018064     0.003480
N    -2.214645    -0.085852    -0.057717
H     1.036995    -1.560560    -1.054883
```

```
 Core  RigidRotor
   SymmetryFactor   1
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 1939.2933
   WellDepth[kJ/mol]    191.80
   WellDepth[kJ/mol]    38.10
   End
   Frequencies[1/cm] 20
 102.2311 145.6162 145.6162
 254.4949 434.1059 496.3907
 602.5216 677.1373 742.8056
 1006.1160 1052.1702 1227.6240
 1405.3450 1468.2553 1480.0857
 1745.1541 2452.8439 3039.2963
 3114.5912 3174.8351
   ZeroEnergy[kJ/mol]        -81.40
   ElectronicLevels[1/cm]                      1
      0        2
End
  !**********************************
 Barrier TS14 INT5 P4
 RRHO
  Geometry[angstrom]            9
C    -0.425636     0.206064     0.067193
O    -0.871318     1.326935    -0.092143
C    -1.245792    -1.060924    -0.058808
H    -1.215910    -1.353930    -1.112469
H    -0.828902    -1.873967     0.534548
C     1.052289    -0.019362     0.007310
N     2.193482    -0.223158    -0.065974
H    -2.275369    -0.855081     0.226532
H    -0.355032     0.187132     1.736063
 Core  RigidRotor
   SymmetryFactor   1
 End
 Rotor Hindered
 Group 4 5 7 8
 Axis 1 3
 Potential[kJ/mol] 24
 0.0
 1.27194123824603
 4.44118267947204
 7.6804566023956
 9.03623703701311
 7.85677705572703
 4.95433425888599
 1.83396735938909
 0.075316847379448
 0.803481914799235
 3.95391396483585
 7.63256836704718
 9.02745085035093
 7.44104272821847
 4.33249759200006
 1.40067037196798
 0.016259223342914
```

```
 0.990109624703408
 4.092344184944
 7.59719837380859
 9.03438387305732
 7.51370597292085
 4.27549580132935
 1.23702725090021
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 1383.6046
   WellDepth[kJ/mol]    92.50
   WellDepth[kJ/mol]    36.90
   End
   Frequencies[1/cm] 20
 174.0690 187.1979 265.0230
 421.5212 506.0490 543.2105
 610.1661 627.6835 728.8824
 1002.8822 1055.3619 1186.0447
 1403.1669 1479.0501 1486.8348
 1742.5459 2258.4587 3054.8681
 3137.3841 3178.0182
   ZeroEnergy[kJ/mol]        -82.60
   ElectronicLevels[1/cm]                      1
      0        2
End
  !***********************************
 Barrier TS15 INT5 P5
 RRHO
  Geometry[angstrom]            9
C    -0.310687     0.527182     0.408540
O    -0.868530     1.354743    -0.294369
C    -1.281700    -1.294700    -0.095820
H    -1.035936    -1.322914    -1.148311
H    -0.764334    -1.986617     0.557108
C     1.047279     0.024054     0.078946
N     2.112807    -0.374459    -0.155865
H    -2.289028    -1.004616     0.168934
H    -0.591439     0.351855     1.457777
 Core  RigidRotor
   SymmetryFactor   1
 End
 Rotor Hindered
 Group 4 5 7 8
 Axis 1 3
 Potential[kJ/mol] 24
 0.0
 0.837700473432463
 2.88165317956669
 4.96293405290399
 5.84277713951649
 4.98632004242865
 2.91552494264156
 0.861326148269313
 0.000788887638976
 0.800416935455104
 2.80723810557623
 4.89198640913928
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```
 5.83928004399593
 5.0764440873165
 3.04796066684208
 0.946550426562126
 0.002563031614521
 0.775205872091355
 2.82282736510102
 4.93997387891793
 5.84173202745631
 4.9779872363624
 2.89136345423071
 0.8405192043342
 End
 Tunneling    Eckart
   ImaginaryFrequency[1/cm] 490.6525
   WellDepth[kJ/mol]    68.20
   WellDepth[kJ/mol]    9.10
   End
   Frequencies[1/cm] 20
 143.6317 150.1111 236.1380
 291.3741 433.0453 593.7990
 614.6141 630.9230 904.2265
 932.4602 1044.3170 1387.4141
 1432.6508 1446.8454 1627.8504
 2263.1225 3000.2002 3108.4727
 3279.5266 3290.5715
   ZeroEnergy[kJ/mol]        -106.90
   ElectronicLevels[1/cm]                    1
      0        2
End
  !***********************************
 Barrier TS16 INT2 P2
 RRHO
  Geometry[angstrom]            9
C     0.436290     0.033779     0.059402
O     0.996474    -1.197203    -0.142723
H     0.329343    -0.013623     1.856427
C     1.172628     1.151842    -0.077762
H     0.693242     2.117949    -0.053825
H     2.248480     1.081821    -0.148338
H     0.412434    -1.880038     0.205614
C    -1.015941     0.089477    -0.006934
N    -2.172698     0.084454    -0.074650
  Core MultiRotor
   SymmetryFactor  1.0
   InterpolationEnergyMax[kJ/mol]  1000
   PotentialEnergySurface[kJ/mol] ./TS16.dat
   InternalRotation
Group 7
Axis 1 2
Symmetry            1
     MassExpansionSize 3
     GridSize         1000
   End
   InternalRotation
Group 5 6 9
Axis 1 4
```

```
 Symmetry            1
      MassExpansionSize 3
      GridSize          1000
    End
    End
  Tunneling    Eckart
    ImaginaryFrequency[1/cm] 1279.0235
    WellDepth[kJ/mol]    146.00
    WellDepth[kJ/mol]    33.20
    End
    Frequencies[1/cm] 20
  189.2045 286.3709 298.5808
  421.2752 514.1961 529.0157
  616.8174 662.7227 696.8953
  807.6498 906.0247 985.7958
  1247.0125  1322.9145 1436.8579
  1645.0141  2383.4583 3195.2091
  3306.7626 3826.3145
    ZeroEnergy[kJ/mol]        -51.90
    ElectronicLevels[1/cm]                      1
       0        2
 End
End
```

6 Arrhenius plots

6.1 *syn*-VyA + CN

Table 97 The Arrhenius-Kooij parameters for the *syn*-VyA + CN addition reaction.

	A/cm^{3}molecule^{-1}s^{-1}	n	E/kJmol^{-1}	rms[a]
s-P1	6.68×10^{-11}	0.37	-114.69	1.09×10^{-12}
s-P2	1.67×10^{-13}	1.02	-484.24	1.08×10^{-14}
s-P3	2.12×10^{-10}	0.19	-3.46	5.32×10^{-13}
s-P4	2.54×10^{-13}	0.39	-139.00	6.44×10^{-15}
s-P5	3.56×10^{-12}	0.57	-214.95	8.98×10^{-14}
s-P6	1.14×10^{-10}	-0.17	187.72	3.79×10^{-12}
s-P7	3.03×10^{-11}	0.59	-236.25	1.02×10^{-12}
s-P1A	5.45×10^{-13}	0.72	-370.04	1.81×10^{-14}

[a] rms stands for root-mean-square deviation of the fit.

Table 98 The NTS parameters for the *syn*-VyA + CN abstraction reaction.

	A/cm^{3}molecule^{-1}s^{-1}	$\varepsilon^{\ddagger}$/kJmol^{-1}	T$_0$/K	rms[a]
s-P2A	1.98×10^{-16}	14171.00	0.01	1.26×10^{-18}
s-P3A	1.14×10^{-13}	14825.34	0.01	5.95×10^{-16}
s-P4A	1.92×10^{-12}	44052.44	-330.96	4.89×10^{-19}

[a] rms stands for root-mean-square deviation of the fit.

6.2 *anti*-VyA + CN

Table 99 The Arrhenius-Kooij parameters for the *anti*-VyA + CN addition reaction.

	A/cm^{3}molecule^{-1}s^{-1}	n	E/kJmol^{-1}	rms[a]
a-P1	2.08×10^{-12}	0.05	69.23	2.39×10^{-14}
a-P2	1.26×10^{-14}	0.38	-103.58	1.39×10^{-16}
a-P3	4.19×10^{10}	0.18	-4.28	3.64×10^{-13}
a-P4	1.77×10^{14}	0.02	70.05	1.60×10^{-16}
a-P5	2.40×10^{-13}	0.07	65.10	3.62×10^{-15}
a-P6	6.21×10^{-12}	-0.47	327.34	3.61×10^{-13}
a-P7	3.69×10^{-13}	0.18	-3.10	4.17×10^{-16}
a-P1A	6.63×10^{-17}	0.59	-224.19	1.80×10^{-16}

[a] rms stands for root-mean-square deviation of the fit.

Table 100 The NTS parameters for the *anti*-VyA + CN abstraction reaction.

	A/cm^{3}molecule^{-1}s^{-1}	$\varepsilon^{\ddagger}$/kJmol^{-1}	T$_0$/K	rms[a]
a-P2A	1.25×10^{-16}	39493.88	-192.94	1.82×10^{-23}
a-P3A	2.85×10^{-16}	8191.73	-0.01	1.44×10^{-17}
a-P4A	9.84×10^{-15}	12951.95	-6.55	4.90×10^{-17}

[a] rms stands for root-mean-square deviation of the fit.

7 $\gamma(\beta)$ vs NTS fitting plots

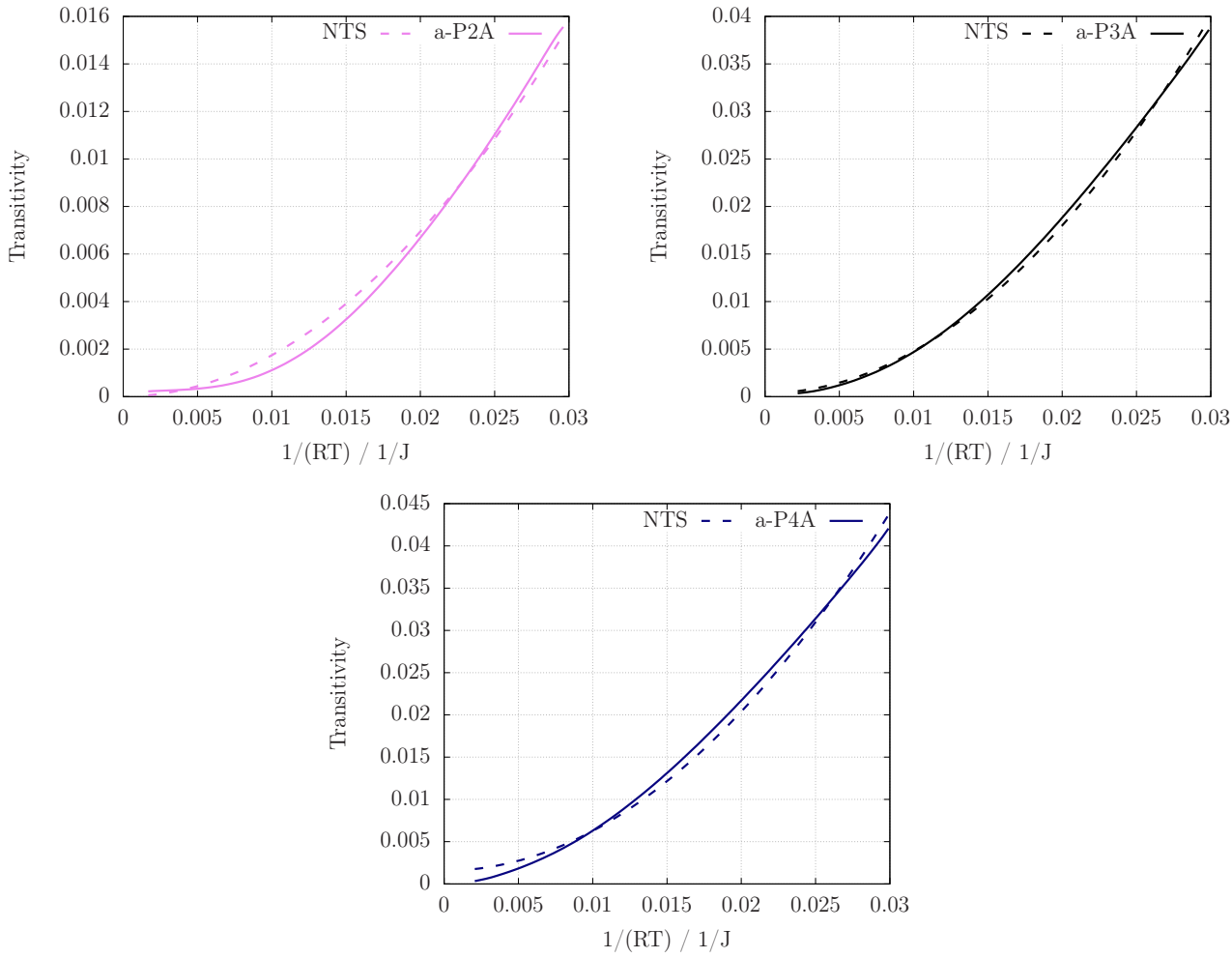

Figure 1 Comparison between NTS fitting function and transitivity data obtained from the kinetic simulations for the abstraction reactions between *anti*-VyA + CN.

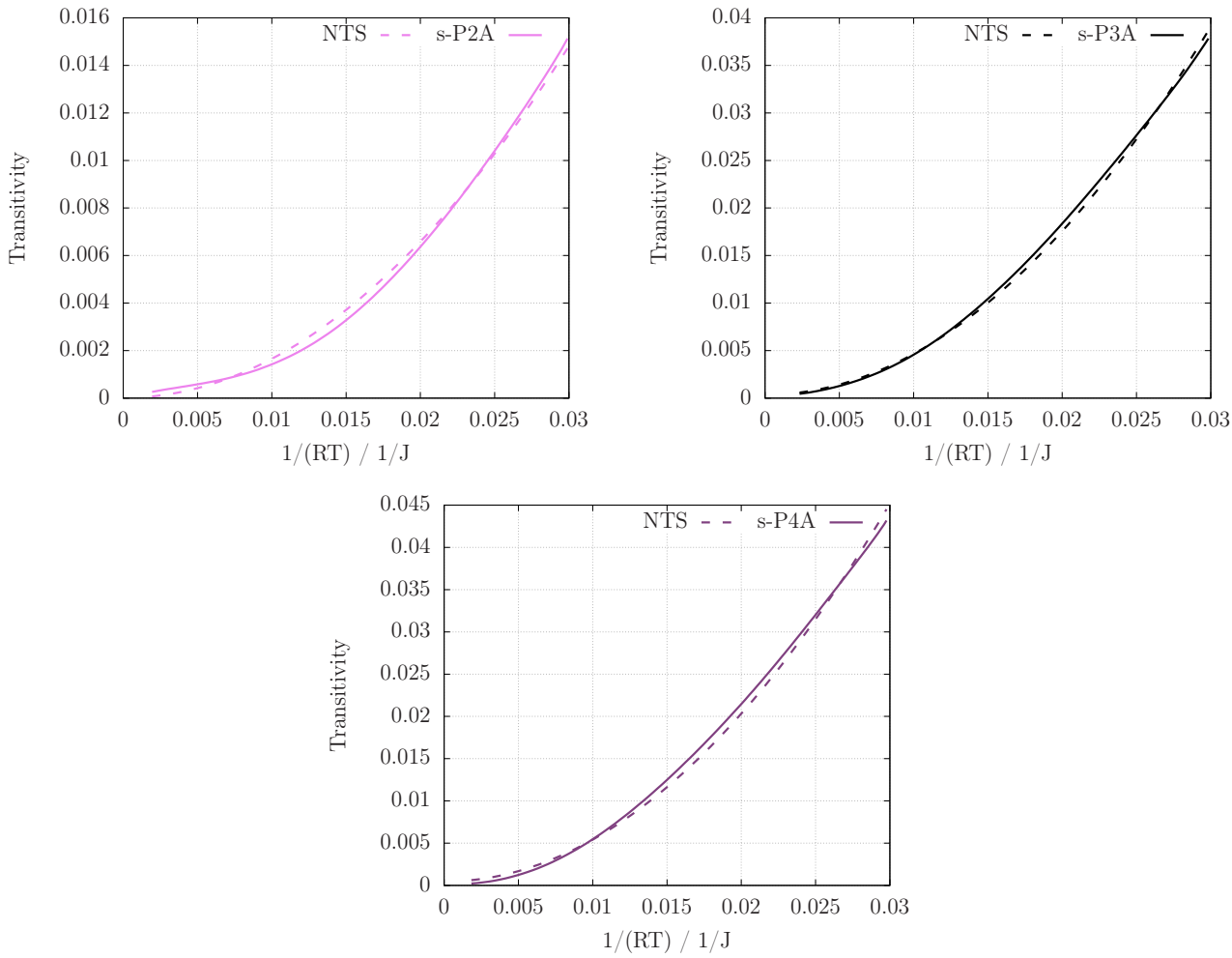

Figure 2 Comparison between NTS fitting function and transitivity data obtained from the kinetic simulations for the abstraction reactions between *syn*-VyA + CN.